

In order to avoid security-related warning messages when switching to secured connection, you may want either to:

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[SwissDrugDesign](#)

[SwissDock](#)

[SwissParam](#)

[SwissSidechain](#)

[SwissBioisostere](#)

[SwissTargetPrediction](#)

[SwissADME](#)

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SwissADME

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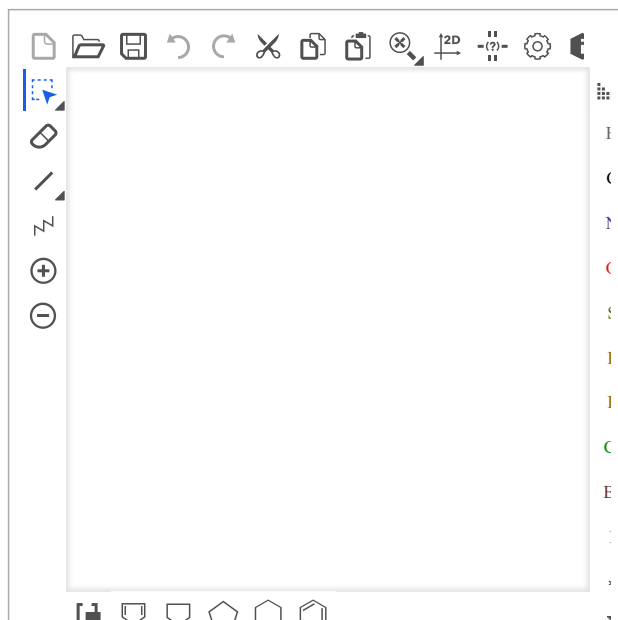
This website allows you to compute physicochemical descriptors as well as to predict ADME parameters, pharmacokinetic properties, druglike nature and medicinal chemistry friendliness of one or multiple small molecules to support drug discovery.

The main article describing the web service and its underlying methodologies is [SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. *Sci. Rep.* \(2017\) 7:42717.](#)

For details about development and validation of iLOG, please refer to this article: [iLOGP: a simple, robust, and efficient description of *n*-octanol/water partition coefficient for drug design using the GB/SA approach. *J. Chem. Inf. Model.* \(2014\) 54\(12\):3284-3301.](#)

For details about development and validation of the BOILED-Egg, please refer to this article: [A BOILED-Egg to predict gastrointestinal absorption and brain penetration of small molecules. *ChemMedChem* \(2016\) 11\(11\):1117-1121.](#)

Developed and maintained by the [Molecular Modeling Group](#) of the SIB | Swiss Institute of Bioinformatics.



Enter a list of SMILES here:

```
CC[C@@H](CO)NCCN[C@@H](CC)CO
CC[C@H](CO)NCCN[C@@H](CC)CO
CC[C@@H](CO)NCCN[C@H](CC)CO
CC(C)[C@@H](CO)NCCN[C@@H](CO)C(C)C
CC(C)[C@@H](CO)NCCN[C@H](CO)C(C)C
CC(C)[C@H](CO)NCCN[C@@H](CO)C(C)C
CC[C@@H](CO)N1CCN(CC(C)(C)O)CC1
CC[C@@H](CO)N1CCN(CC(C)(C)O)CC1
C[C@@H](O)CN1CCN(C[C@@H](C)O)CC1
C[C@H](O)CN1CCN(C[C@H](C)O)CC1
C[C@@H](O)CN1CCN(C[C@H](C)O)CC1
C[C@@H](O)CN(CCO)CCN(C[C@@H](C)O)C[C@@H](C)O
C[C@H]1CN(CCO)[C@H](C)CN1CCO
C[C@@H](O)CN(CCO)CCN(CCO)C[C@@H](C)O
C[C@H]1CN(CCO)[C@H](C)CN1CCO
C[C@@H]1CN(CCO)[C@H](C)CN1CCO
C[C@H](O)CN(CCO)CCN(C[C@@H](C)O)C[C@@H](C)O
C[C@@H](O)CN(CCN(C[C@H](C)O)C[C@H](C)O)C[C@@H](C)O
C[C@@H](O)CN(CCN(C[C@H](C)O)C[C@H](C)O)C[C@@H](C)O
C[C@@H](O)CN(CCO)CCN(CCO)C[C@H](C)O
```

Fill with an example

Clear

Run!

Show BOILED-Egg

Retrieve data: POWERED BY ChemAxon

Molecule 1

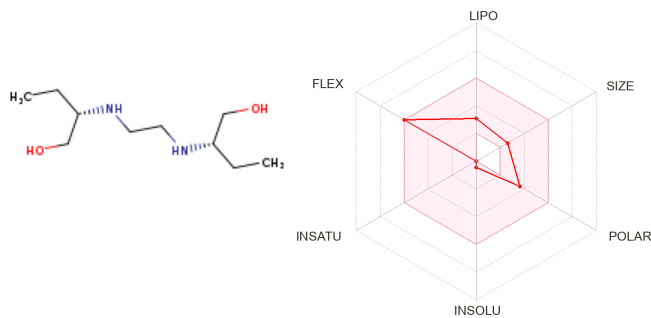


Log *S* (ESOL)

Water Solubility

-0.46

[ESOL: Topological method implemented from](#)



SMILES CC[C@H](NCCN[C@H](CO)CC)CO

Physicochemical Properties	
Formula	C10H24N2O2
Molecular weight	204.31 g/mol
Num. heavy atoms	14
Num. arom. heavy atoms	0
Fraction Csp3	1.00
Num. rotatable bonds	9
Num. H-bond acceptors	4
Num. H-bond donors	4
Molar Refractivity	58.11
TPSA	

Topological Polar Surface Area: 64.52 Å²
 Calculated from [Ertl P. et al. 2000 J. Med. Chem.](#)

Lipophilicity
 Log $P_{o/w}$ (iLOGP)

iLOGP: in-house physics-based method implemented from [Daina A et al. 2014 J. Chem. Inf. Model.](#) 2.47

XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry. -0.08

WLOGP: Atomistic method implemented from [Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.](#) -0.29

MLOGP: Topological method implemented from [Moriguchi I. et al. 1992 Chem. Pharm. Bull.](#) and [Moriguchi I. et al. 1994 Chem. Pharm. Bull.](#) 0.18

[Delaney JS. 2004 J. Chem. Inf. Model.](#)

Solubility 7.05e+01 mg/ml ; 3.45e-01 mol/l

Class

Solubility class: Log S scale
 Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Log S (Ali)

Ali: Topological method implemented from [Ali J. et al. 2012 J. Chem. Inf. Model.](#) -0.82

Solubility 3.07e+01 mg/ml ; 1.50e-01 mol/l

Class

Solubility class: Log S scale
 Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Log S (SILICOS-IT)

SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com> -2.14

Solubility 1.48e+00 mg/ml ; 7.24e-03 mol/l

Class

Solubility class: Log S scale
 Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Pharmacokinetics

GI absorption

Gastrointestinal absorption: according to the white of the BOILED-Egg High

BBB permeant

BBB permeation: according to the yolk of the BOILED-Egg No

P-gp substrate

P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 No

[Lipinski PA. et al. 2001
Adv. Drug. Deliv. Rev.](#)
Log $P_{o/w}$ (SILICOS-IT)

0.72

SILICOS-IT: Hybrid
fragmental/topological
method calculated by
FILTER-IT program,
version 1.0.2, courtesy
of SILICOS-IT,
[http://www.silicos-
it.com](http://www.silicos-
it.com)

Consensus Log $P_{o/w}$

Consensus Log $P_{o/w}$:
Average of all five
predictions

0.72

0.60

External: ACC=0.88 /
AUC=0.94

CYP1A2 inhibitor

Cytochrome P450 1A2

inhibitor: SVM model
built on 9145 molecules
(training set)

and tested on 3000
molecules (test set)

10-fold CV: ACC=0.83 /

AUC=0.90

External: ACC=0.84 /

AUC=0.91

No

CYP2C19 inhibitor

Cytochrome P450

2C19 inhibitor: SVM

model built on 9272
molecules (training set)

and tested on 3000
molecules (test set)

10-fold CV: ACC=0.80 /

AUC=0.86

External: ACC=0.80 /

AUC=0.87

No

CYP2C9 inhibitor

Cytochrome P450 2C9

inhibitor: SVM model

built on 5940 molecules
(training set)

and tested on 2075
molecules (test set)

10-fold CV: ACC=0.78 /

AUC=0.85

External: ACC=0.71 /

AUC=0.81

No

CYP2D6 inhibitor

Cytochrome P450 2D6

inhibitor: SVM model

built on 3664 molecules
(training set)

and tested on 1068
molecules (test set)

10-fold CV: ACC=0.79 /

AUC=0.85

External: ACC=0.81 /

AUC=0.87

No

CYP3A4 inhibitor

Cytochrome P450 3A4

inhibitor: SVM model

built on 7518 molecules
(training set)

and tested on 2579
molecules (test set)

10-fold CV: ACC=0.77 /

AUC=0.85

External: ACC=0.78 /

AUC=0.86

No

Log K_p (skin
permeation)

Skin permeation:

QSPR model
implemented from
Potts RO and Guy RH.
1992 Pharm. Res.

-7.60 cm/s

Druglikeness

Lipinski **Lipinski (Pfizer) filter:**

implemented from

[Lipinski CA. et al. 2001](#)[Adv. Drug Deliv. Rev.](#)

Yes; 0 violation

[MW < 500](#)[MLOGP < 4.15](#)[N or O < 10](#)[NH or OH < 5](#)Ghose **Ghose filter:**

implemented from

[Ghose AK. et al. 1999 J.](#)[Comb. Chem.](#)

Yes

[160 < MW < 480](#)[-0.4 < WLOGP < 5.6](#)[40 < MR < 130](#)[20 < atoms < 70](#)Veber **Veber (GSK) filter:**

implemented from

[Veber DE. et al. 2002 J.](#)[Med. Chem.](#)


Yes

[Rotatable bonds < 10](#)[TPSA < 140](#)Egan **Egan (Pharmacia)****filter:** implemented

from

[Egan WJ. et al. 2000 J.](#)[Med. Chem.](#)


Yes

[WLOGP < 5.88](#)[TPSA < 131.6](#)Muegge **Muegge (Bayer) filter:**

implemented from

[Muegge I. et al. 2001 J.](#)[Med. Chem.](#)[200 < MW < 600](#)[-2 < XLOGP < 5](#)[TPSA < 150](#)

Yes

[Num. rings < 7](#)[Num. carbon > 4](#)[Num. heteroatoms > 1](#)[Num. rotatable bonds <](#)[15](#)[H-bond acc. < 10](#)[H-bond don. < 5](#)Bioavailability Score **Abbott Bioavailability****Score:** Probability of F[> 10% in rat](#)

0.55

implemented from

[Martin YC. 2005 J.](#)[Med. Chem.](#)

Medicinal Chemistry

PAINS **Pan Assay Interference****Structures:**

implemented from

[Baell JB. & Holloway](#)[GA. 2010 J. Med.](#)[Chem.](#)

0 alert

Brenk

Structural Alert:

implemented from [Brenk R. et al. 2008 ChemMedChem](#) 0 alert

Leadlikeness

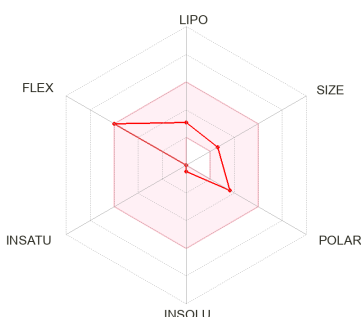
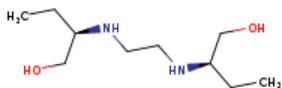
Leadlikeness:

implemented from [Teague SJ. 1999 Angew. Chem. Int. Ed.](#) No; 2 violations: MW<250, Rotors>7
[250 < MW < 350](#)
[XLOGP < 3.5](#)
[Num. rotatable bonds < 7](#)

Synthetic accessibility

Synthetic accessibility:

score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penalties, trained on 12'782'590 molecules and tested on 40 external molecules ($r^2 = 0.94$) 2.40

Molecule 2

SMILES
S CC[C@H](NCCN[C@H](CO)CC)CO

Physicochemical Properties

Formula C10H24N2O2
 Molecular weight 204.31 g/mol
 Num. heavy atoms 14
 Num. arom. heavy atoms 0
 Fraction Csp3 1.00
 Num. rotatable bonds 9
 Num. H-bond acceptors 4
 Num. H-bond donors 4
 Molar Refractivity 58.11
 TPSA

Topological Polar

Surface Area: 64.52 Å²
 Calculated from [Ertl P. et al. 2000 J. Med. Chem.](#)

Lipophilicity

Log S (ESOL)

ESOL: Topological method implemented from [Delaney JS. 2004 J. Chem. Inf. Model.](#)

Water Solubility

-0.46

Solubility Class

7.05e+01 mg/ml ; 3.45e-01 mol/l

Solubility class: Log S scale

[Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly](#) Very soluble

Log S (Ali)

Ali: Topological method implemented from [Ali J. et al. 2012 J. Chem. Inf. Model.](#)


-0.82


Solubility Class


3.07e+01 mg/ml ; 1.50e-01 mol/l


Solubility class: Log S scale


[Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly](#) Very soluble


Log $P_{o/w}$ (iLOGP) 
iLOGP: in-house physics-based method implemented from [Daina A et al. 2014 J. Chem. Inf. Model.](#) 2.38


Log $P_{o/w}$ (XLOGP3) 
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry. -0.08


Log $P_{o/w}$ (WLOGP) 
WLOGP: Atomistic method implemented from [Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.](#) -0.29


Log $P_{o/w}$ (MLOGP) 
MLOGP: Topological method implemented from [Moriguchi I. et al. 1992 Chem. Pharm. Bull.](#) [Moriguchi I. et al. 1994 Chem. Pharm. Bull.](#) [Lipinski PA, et al. 2001 Adv. Drug. Deliv. Rev.](#) 0.18


Log $P_{o/w}$ (SILICOS-IT) 
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com> 0.72


Consensus Log $P_{o/w}$ 
Consensus Log $P_{o/w}$: Average of all five predictions 0.58


Log S (SILICOS-IT) 
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com> -2.14


Solubility 1.48e+00 mg/ml ; 7.24e-03 mol/l
 Class 
Solubility class: Log S scale Insoluble < -10 < Poorly Soluble < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

GI absorption 
Gastrointestinal absorption: according to the white of the BOILED-Egg High

BBB permeant 
BBB permeation: according to the yolk of the BOILED-Egg No

P-gp substrate 
P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94 No

CYP1A2 inhibitor 
Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91 No

CYP2C19 inhibitor 
Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87 No

CYP2C9 inhibitor ⓘ

Cytochrome P450 2C9**inhibitor:** SVM model

built on 5940 molecules

(training set)

and tested on 2075 No

molecules (test set)

10-fold CV: ACC=0.78 /

AUC=0.85

External: ACC=0.71 /

AUC=0.81

CYP2D6 inhibitor ⓘ

Cytochrome P450 2D6**inhibitor:** SVM model

built on 3664 molecules

(training set)

and tested on 1068 No

molecules (test set)

10-fold CV: ACC=0.79 /

AUC=0.85

External: ACC=0.81 /

AUC=0.87

CYP3A4 inhibitor ⓘ

Cytochrome P450 3A4**inhibitor:** SVM model

built on 7518 molecules

(training set)

and tested on 2579 No

molecules (test set)

10-fold CV: ACC=0.77 /

AUC=0.85

External: ACC=0.78 /

AUC=0.86

Log K_p (skin
permeation) ⓘ**Skin permeation:**

QSPR model

-7.60 cm/s

implemented from

Potts RO and Guy RH.

1992 Pharm. Res.

Druglikeness

Lipinski ⓘ

Lipinski (Pfizer) filter:

implemented from

Lipinski CA. et al. 2001

Adv. Drug Deliv. Rev. Yes; 0 violation

MW < 500

MLOGP < 4.15

N or O < 10

NH or OH < 5

Ghose ⓘ

Ghose filter:

implemented from

Ghose AK. et al. 1999 J.

Comb. Chem. Yes

160 < MW < 480

-0.4 < WLOGP < 5.6

40 < MR < 130

20 < atoms < 70

Veber ⓘ

Yes

Veber (GSK) filter:

implemented from

Veber DE. et al. 2002 J.

Med. Chem.

[Rotatable bonds < 10](#)
[TPSA < 140](#)

Egan

Egan (Pharmacia)

filter: [implemented](#)

[from](#)

[Egan W.J. et al. 2000 J.](#) Yes

[Med. Chem.](#)

[WLOGP < 5.88](#)

[TPSA < 131.6](#)

Muegge

Muegge (Bayer) filter:

[implemented from](#)

[Muegge I. et al. 2001 J.](#)

[Med. Chem.](#)

[200 < MW < 600](#)

[-2 < XLOGP < 5](#)

[TPSA < 150](#) Yes

[Num. rings < 7](#)

[Num. carbon > 4](#)

[Num. heteroatoms > 1](#)

[Num. rotatable bonds <](#)

[15](#)

[H-bond acc. < 10](#)

[H-bond don. < 5](#)

Bioavailability Score

Abbott Bioavailability

Score: [Probability of F](#)

[> 10% in rat](#) 0.55

[implemented from](#)

[Martin Y.C. 2005 J.](#)

[Med. Chem.](#)

Medicinal Chemistry

PAINS

Pan Assay Interference

Structures:

[implemented from](#) 0 alert

[Baell JB. & Holloway](#)

[GA. 2010 J. Med.](#)

[Chem.](#)

Brenk

Structural Alert:

[implemented from](#) 0 alert

[Brenk R. et al. 2008](#)

[ChemMedChem](#)

Leadlikeness

Leadlikeness:

[implemented from](#)

[Teague S.J. 1999 Angew.](#)

[Chem. Int. Ed.](#) No; 2 violations: MW<250, Rotors>7

[250 < MW < 350](#)

[XLOGP < 3.5](#)

[Num. rotatable bonds <](#)

[7](#)

Synthetic accessibility 2.40

Synthetic accessibility

score: [from 1 \(very](#)

[easy\) to 10 \(very](#)

[difficult\)](#)

[based on 1024](#)

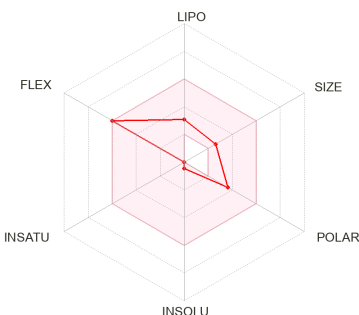
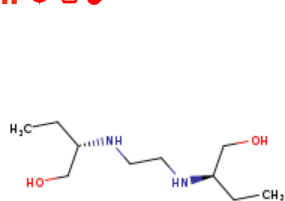
[fragmental contributions](#)

[\(FP2\) modulated by size](#)

[and complexity penalties.](#)

trained on 12'782'590
molecules and tested on
40 external molecules
($r^2 = 0.94$)

Molecule 3



SMILES
S CC[C@H](NCCN[C@@H](CO)CC)CO

Physicochemical Properties

Formula C10H24N2O2
Molecular weight 204.31 g/mol
Num. heavy atoms 14
Num. arom. heavy atoms 0
Fraction Csp3 1.00
Num. rotatable bonds 9
Num. H-bond acceptors 4
Num. H-bond donors 4
Molar Refractivity 58.11
TPSA

Topological Polar Surface Area:
Calculated from
Ertl P. et al. 2000 J. Med. Chem.
64.52 Å²

Lipophilicity

Log $P_{o/w}$ (iLOGP)
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.
2.32

Log $P_{o/w}$ (XLOGP3)
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.
-0.08

Log $P_{o/w}$ (WLOGP)
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.
-0.29

Log S (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.
-0.46

Solubility Class
7.05e+01 mg/ml ; 3.45e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly
Very soluble

Log S (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.
-0.82

Solubility Class
3.07e+01 mg/ml ; 1.50e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly
Very soluble

Log S (SILICOS-IT)

SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>
-2.14

Solubility Class
1.48e+00 mg/ml ; 7.24e-03 mol/l


Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly
Soluble

Water Solubility


Pharmacokinetics

GI absorption


Gastrointestinal absorption: according to the white of the BOILED-Egg
High

Log $P_{o/w}$ (MLOGP) **MLOGP: Topological method implemented from**[Moriguchi I. et al. 1992 Chem. Pharm. Bull.](#)[Moriguchi I. et al. 1994 Chem. Pharm. Bull.](#)[Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.](#)


0.18

Log $P_{o/w}$ (SILICOS-IT) **SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>**


0.72

Consensus Log $P_{o/w}$ **Consensus Log $P_{o/w}$: Average of all five predictions**


0.57

BBB permeant **BBB permeation:** [according to the yolk of the BOILED-Egg](#)


No

P-gp substrate **P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94**


No

CYP1A2 inhibitor **Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91**


No

CYP2C19 inhibitor **Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87**


No

CYP2C9 inhibitor **Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set). 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81**

No


CYP2D6 inhibitor **Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set). 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87**

No

CYP3A4 inhibitor **Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set)**

No

and tested on 2579
 molecules (test set)
 10-fold CV: ACC=0.77 /
 AUC=0.85
 External: ACC=0.78 /
 AUC=0.86

Log K_p (skin
 permeation) 

Skin permeation:

[QSPR model](#) -7.60 cm/s
 implemented from
[Potts RO and Guy RH.](#)
[1992 Pharm. Res.](#)

Druglikeness

Lipinski 

Lipinski (Pfizer) filter:

implemented from
[Lipinski CA. et al. 2001](#)
[Adv. Drug Deliv. Rev.](#) Yes; 0 violation
 MW < 500
 MLOGP < 4.15
 N or O < 10
 NH or OH < 5

Ghose 

Ghose filter:

implemented from
[Ghose AK. et al. 1999 J.](#)
[Comb. Chem.](#) Yes
 160 < MW < 480
 -0.4 < WLOGP < 5.6
 40 < MR < 130
 20 < atoms < 70

Veber 


Veber (GSK) filter:

implemented from
[Veber DF. et al. 2002 J.](#) Yes
[Med. Chem.](#)
 Rotatable bonds < 10
 TPSA < 140

Egan 

**Egan (Pharmacia)
 filter:** implemented

from
[Egan WJ. et al. 2000 J.](#) Yes
[Med. Chem.](#)
 WLOGP < 5.88
 TPSA < 131.6

Muegge 

Muegge (Bayer) filter:

implemented from
[Muegge I. et al. 2001 J.](#)
[Med. Chem.](#)
 200 < MW < 600
 -2 < XLOGP < 5
 TPSA < 150 Yes
 Num. rings < 7
 Num. carbon > 4
 Num. heteroatoms > 1
 Num. rotatable bonds <
 15
 H-bond acc. < 10
 H-bond don. < 5

Bioavailability Score

Abbott Bioavailability:**Score:** Probability of F

> 10% in rat 0.55

implemented from

[Martin YC. 2005 J.](#)[Med. Chem.](#)

Medicinal Chemistry

PAINS

Pan Assay Interference**Structures:**

implemented from 0 alert

[Baell JB. & Holloway](#)[GA. 2010 J. Med.](#)[Chem.](#)

Brenk

Structural Alert:

implemented from 0 alert

[Brenk R. et al. 2008](#)[ChemMedChem](#)

Leadlikeness

Leadlikeness:

implemented from

[Teague SJ. 1999 Angew.](#)[Chem. Int. Ed.](#)

No; 2 violations: MW<250, Rotors>7

[250 < MW < 350](#)[XLOGP < 3.5](#)[Num. rotatable bonds <](#)[7](#)

Synthetic accessibility

Synthetic accessibility**score:** from 1 (very

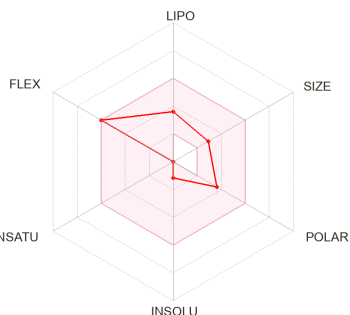
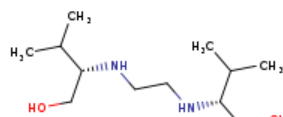
easy) to 10 (very

difficult)

based on 1024

[fragmental contributions](#) 2.40[\(FP2\) modulated by size](#)[and complexity penalties.](#)[trained on 12'782'590](#)[molecules and tested on](#)[40 external molecules](#)[\(r² = 0.94\)](#)

Molecule 4



Log S (ESOL)

ESOL: Topological method implemented from[Delaney JS. 2004 J.](#)[Chem. Inf. Model.](#)

Water Solubility

-1.18

Solubility

1.52e+01 mg/ml ; 6.54e-02 mol/l

Class

Solubility class: Log S scale[Insoluble < -10 < Poorly](#) Very soluble[< -6 < Moderately < -4](#)[< Soluble < -2 Very < 0](#)[< Highly](#)SMILES OC[C@H](C(C)C)NCCN[C@H](C(C)C)CO

Physicochemical Properties


Formula C₁₂H₂₈N₂O₂

Molecular weight 232.36 g/mol


Num. heavy atoms 16

Num. arom. heavy atoms	0	Log <i>S</i> (Ali)	
Fraction Csp3	1.00	Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-1.73
Num. rotatable bonds	9		
Num. H-bond acceptors	4		
Num. H-bond donors	4		
Molar Refractivity	67.72	Solubility	4.37e+00 mg/ml ; 1.88e-02 mol/l
TPSA		Class	
Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	64.52 Å ²	Solubility class: Log <i>S</i> scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Very soluble
	Lipophilicity		
Log <i>P</i> _{o/w} (iLOGP)		Log <i>S</i> (SILICOS-IT)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.77	SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-2.20
Log <i>P</i> _{o/w} (XLOGP3)			
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.	0.79	Solubility	1.46e+00 mg/ml ; 6.27e-03 mol/l
		Class	
Log <i>P</i> _{o/w} (WLOGP)		Solubility class: Log <i>S</i> scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	0.20		
			Pharmacokinetics
Log <i>P</i> _{o/w} (MLOGP)		GI absorption	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	0.75	Gastrointestinal absorption: according to the white of the BOILED-Egg	High
		BBB permeant	
Log <i>P</i> _{o/w} (SILICOS-IT)		BBB permeation: according to the yolk of the BOILED-Egg	No
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	1.23	P-gp substrate	
		P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
Consensus Log <i>P</i> _{o/w}		CYP1A2 inhibitor	No
Consensus Log <i>P</i>_{o/w}: Average of all five predictions	1.15	Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.83 / AUC=0.90	


[External: ACC=0.84 / AUC=0.91](#)

CYP2C19 inhibitor 


Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) No
 10-fold CV: ACC=0.80 / AUC=0.86
 External: ACC=0.80 / AUC=0.87

CYP2C9 inhibitor 


Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) No
 10-fold CV: ACC=0.78 / AUC=0.85
 External: ACC=0.71 / AUC=0.81

CYP2D6 inhibitor 

Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) No
 10-fold CV: ACC=0.79 / AUC=0.85
 External: ACC=0.81 / AUC=0.87

CYP3A4 inhibitor 

Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) No
 10-fold CV: ACC=0.77 / AUC=0.85
 External: ACC=0.78 / AUC=0.86

Log K_p (skin permeation) 

Skin permeation: QSPR model implemented from Potts RO and Guy RH. 1992 Pharm. Res. -7.16 cm/s

Druglikeness

Lipinski 

Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. Yes; 0 violation
 MW < 500
 MLOGP < 4.15
 N or O < 10
 NH or OH < 5

Ghose ?

Ghose filter:

implemented from

[Ghose AK. et al. 1999 J.](#)[Comb. Chem.](#)

Yes

[160 < MW < 480](#)[-0.4 < WLOGP < 5.6](#)[40 < MR < 130](#)[20 < atoms < 70](#)

Veber ?

Veber (GSK) filter:

implemented from

[Veber DF. et al. 2002 J.](#)[Med. Chem.](#)

Yes

[Rotatable bonds < 10](#)[TPSA < 140](#)

Egan ?

Egan (Pharmacia)**filter:** implemented

from

[Egan WJ. et al. 2000 J.](#)[Med. Chem.](#)

Yes

[WLOGP < 5.88](#)[TPSA < 131.6](#)

Muegge ?

Muegge (Bayer) filter:

implemented from

[Muegge I. et al. 2001 J.](#)[Med. Chem.](#)[200 < MW < 600](#)[-2 < XLOGP < 5](#)[TPSA < 150](#)

Yes

[Num. rings < 7](#)[Num. carbon > 4](#)[Num. heteroatoms > 1](#)[Num. rotatable bonds <](#)[15](#)[H-bond acc. < 10](#)[H-bond don. < 5](#)

Bioavailability Score ?

Abbott Bioavailability**Score:** Probability of F[> 10% in rat](#)

0.55

implemented from

[Martin YC. 2005 J.](#)[Med. Chem.](#)

Medicinal Chemistry

PAINS ?

Pan Assay Interference**Structures:**

implemented from

0 alert

[Baell JB. & Holloway.](#)[GA. 2010 J. Med.](#)[Chem.](#)

Brenk ?

Structural Alert:

implemented from

0 alert

[Brenk R. et al. 2008](#)[ChemMedChem](#)

Leadlikeness ?

No; 2 violations: MW<250, Rotors>7

Leadlikeness:

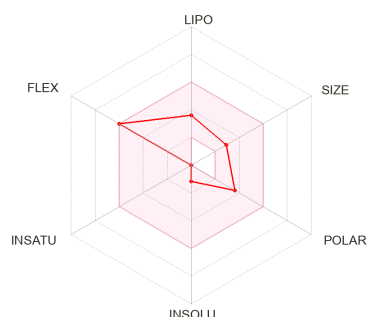
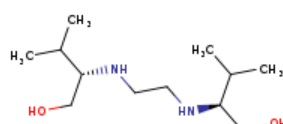
implemented from

Teague SJ. 1999 Angew.
Chem. Int. Ed.
250 < MW < 350
XLOGP < 3.5
Num. rotatable bonds <
7

Synthetic accessibility [?]

Synthetic accessibility
score: from 1 (very
easy) to 10 (very
difficult)
based on 1024
fragmental contributions 2.61
(FP2) modulated by size
and complexity penalties,
trained on 12'782'590
molecules and tested on
40 external molecules
($r^2 = 0.94$)

Molecule 5



SMILE OC[C@H](C(C)C)NCCN[C@@H](C(C)C)CO

Physicochemical Properties

Formula	C12H28N2O2
Molecular weight	232.36 g/mol
Num. heavy atoms	16
Num. arom. heavy atoms	0
Fraction Csp3	1.00
Num. rotatable bonds	9
Num. H-bond acceptors	4
Num. H-bond donors	4
Molar Refractivity	67.72
TPSA [?]	

Topological Polar Surface Area: 64.52 Å²
Calculated from
Ertl P. et al. 2000 J.
Med. Chem.

Lipophilicity
Log $P_{o/w}$ (iLOGP) [?]

iLOGP: in-house
physics-based method
implemented from
Daina A et al. 2014 J.
Chem. Inf. Model. 2.67

Log $P_{o/w}$ (XLOGP3) [?] 0.79

XLOGP3: Atomistic
and knowledge-based

Log S (ESOL) [?]

ESOL: Topological
method implemented
from
Delaney JS. 2004 J.
Chem. Inf. Model.

Solubility
Class [?]

**Solubility class: Log S
scale**
Insoluble < -10 < Poorly
< -6 < Moderately < -4
< Soluble < -2 Very < 0
< Highly

Log S (Ali) [?]

Ali: Topological method
implemented from
Ali J. et al. 2012 J.
Chem. Inf. Model.

Solubility
Class [?]

**Solubility class: Log S
scale**
Insoluble < -10 < Poorly
< -6 < Moderately < -4
< Soluble < -2 Very < 0
< Highly

Log S (SILICOS-IT) [?]

SILICOS-IT:
Fragmental method
calculated by
FILTER-IT program,
version 1.0.2, courtesy
of SILICOS-IT,
[http://www.silicos-
it.com](http://www.silicos-it.com) -2.20

Solubility

Water Solubility

-1.18

1.52e+01 mg/ml ; 6.54e-02 mol/l

Very soluble

-1.73

4.37e+00 mg/ml ; 1.88e-02 mol/l

Very soluble

-2.20

1.46e+00 mg/ml ; 6.27e-03 mol/l

[method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.](#)

Log $P_{o/w}$ (WLOGP) [?]

WLOGP: Atomistic method implemented from

0.20

[Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.](#)

Log $P_{o/w}$ (MLOGP) [?]

MLOGP: Topological method implemented from

0.75

[Moriguchi I. et al. 1992 Chem. Pharm. Bull.](#)
[Moriguchi I. et al. 1994 Chem. Pharm. Bull.](#)
[Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.](#)

Log $P_{o/w}$ (SILICOS-IT) [?]

SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>

1.23

Consensus Log $P_{o/w}$ [?]

Consensus Log $P_{o/w}$: Average of all five predictions

1.13

Class [?]

Solubility class: Log S

scale

[Insoluble < -10 < Poorly Soluble < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly](#)

Pharmacokinetics

GI absorption [?]

Gastrointestinal absorption: according to the white of the BOILED-Egg High

BBB permeant [?]

BBB permeation: according to the yolk of the BOILED-Egg No

P-gp substrate [?]

P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). No
10-fold CV: ACC=0.72 / AUC=0.77
External: ACC=0.88 / AUC=0.94

CYP1A2 inhibitor [?]


Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). No
10-fold CV: ACC=0.83 / AUC=0.90
External: ACC=0.84 / AUC=0.91

CYP2C19 inhibitor [?]

Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set). No
10-fold CV: ACC=0.80 / AUC=0.86
External: ACC=0.80 / AUC=0.87

CYP2C9 inhibitor [?]

Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set). No
10-fold CV: ACC=0.78 / AUC=0.85
External: ACC=0.71 / AUC=0.81

CYP2D6 inhibitor **Cytochrome P450 2D6****inhibitor:** [SVM model](#)[built on 3664 molecules](#)[\(training set\)](#)

and tested on 1068 No


[molecules \(test set\)](#)

10-fold CV: ACC=0.79 /

AUC=0.85

External: ACC=0.81 /

AUC=0.87

CYP3A4 inhibitor **Cytochrome P450 3A4****inhibitor:** [SVM model](#)[built on 7518 molecules](#)[\(training set\)](#)

and tested on 2579 No


[molecules \(test set\)](#)

10-fold CV: ACC=0.77 /

AUC=0.85

External: ACC=0.78 /


AUC=0.86

Log K_p (skin
permeation) **Skin permeation:**[QSPR model](#)

-7.16 cm/s

[implemented from](#)[Potts RO and Guy RH.](#)[1992 Pharm. Res.](#)

Druglikeness

Lipinski **Lipinski (Pfizer) filter:**[implemented from](#)[Lipinski CA. et al. 2001](#)[Adv. Drug Deliv. Rev.](#)

Yes; 0 violation

[MW < 500](#)[MLOGP < 4.15](#)[N or O < 10](#)[NH or OH < 5](#)Ghose **Ghose filter:**[implemented from](#)[Ghose AK. et al. 1999 J.](#)[Comb. Chem.](#)

Yes


[160 < MW < 480](#)[-0.4 < WLOGP < 5.6](#)[40 < MR < 130](#)[20 < atoms < 70](#)Veber **Veber (GSK) filter:**[implemented from](#)[Veber DF. et al. 2002 J.](#)[Med. Chem.](#)

Yes


[Rotatable bonds < 10](#)[TPSA < 140](#)Egan **Egan (Pharmacia)****filter:** [implemented](#)[from](#)[Egan WJ. et al. 2000 J.](#)[Med. Chem.](#)

Yes

[WLOGP < 5.88](#)[TPSA < 131.6](#)

Muegge **Muegge (Bayer) filter:**

implemented from
[Muegge I. et al. 2001 J. Med. Chem.](#)
 $200 < MW < 600$
 $-2 < XLOGP < 5$
 $TPSA < 150$ Yes
 $Num. rings < 7$
 $Num. carbon > 4$
 $Num. heteroatoms > 1$
 $Num. rotatable bonds < 15$
 $H-bond acc. < 10$
 $H-bond don. < 5$

Bioavailability Score **Abbott Bioavailability**

Score: Probability of F
 $> 10\%$ in rat 0.55
 implemented from
[Martin YC. 2005 J. Med. Chem.](#)

Medicinal Chemistry

PAINS **Pan Assay Interference**


Structures:
 implemented from 0 alert
[Baell JB. & Holloway GA. 2010 J. Med. Chem.](#)

Brenk **Structural Alert:**

implemented from 0 alert
[Brenk R. et al. 2008 ChemMedChem](#)

Leadlikeness **Leadlikeness:**

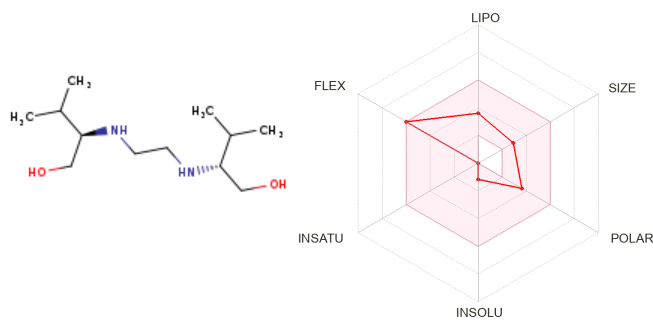
implemented from
[Teague SJ. 1999 Angew. Chem. Int. Ed.](#) No; 2 violations: MW<250, Rotors>7
 $250 < MW < 350$
 $XLOGP < 3.5$
 $Num. rotatable bonds < 7$

Synthetic accessibility **Synthetic accessibility**

score: from 1 (very easy) to 10 (very difficult)
 based on 1024
[fragmental contributions \(FP2\) modulated by size and complexity penalties, trained on 12'782'590 molecules and tested on 40 external molecules](#) 2.61
 $(r^2 = 0.94)$

Molecule 6

Water Solubility 



SMILES OC[C@@H](C(C)C)NCCN[C@H](C(C)C)CO

Physicochemical Properties

Formula	C12H28N2O2
Molecular weight	232.36 g/mol
Num. heavy atoms	16
Num. arom. heavy atoms	0
Fraction Csp3	1.00
Num. rotatable bonds	9
Num. H-bond acceptors	4
Num. H-bond donors	4
Molar Refractivity	67.72
TPSA	

Topological Polar Surface Area: 64.52 Å²
 Calculated from Ertl P. et al. 2000 J. Med. Chem.

Lipophilicity

Log $P_{o/w}$ (iLOGP) 2.72
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.

Log $P_{o/w}$ (XLOGP3) 0.79
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.

Log $P_{o/w}$ (WLOGP) 0.20
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.

Log $P_{o/w}$ (MLOGP) 0.75
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull.

Log S (ESOL) -1.18
ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.

Solubility Class 1.52e+01 mg/ml ; 6.54e-02 mol/l

Solubility class: Log S scale
 Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Log S (Ali) -1.73
Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.

Solubility Class 4.37e+00 mg/ml ; 1.88e-02 mol/l

Solubility class: Log S scale
 Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Log S (SILICOS-IT) -2.20
SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>

Solubility Class 1.46e+00 mg/ml ; 6.27e-03 mol/l

Solubility class: Log S scale
 Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Pharmacokinetics

GI absorption High
Gastrointestinal absorption: according to the white of the BOILED-Egg

BBB permeant No
BBB permeation: according to the yolk of the BOILED-Egg

P-gp substrate No
P-glycoprotein substrate: SVM model built on 1033 molecules

[Lipinski PA. et al. 2001
Adv. Drug. Deliv. Rev.](#)
Log $P_{o/w}$ (SILICOS-IT)

SILICOS-IT: Hybrid
fragmental/topological
method calculated by
FILTER-IT program, 1.23
version 1.0.2, courtesy
of SILICOS-IT,
[http://www.silicos-
it.com](http://www.silicos-
it.com)

Consensus Log $P_{o/w}$

Consensus Log $P_{o/w}$: 1.14
[Average of all five
predictions](#)

(training set)
and tested on 415
molecules (test set)
10-fold CV: ACC=0.72 /
AUC=0.77
External: ACC=0.88 /
AUC=0.94
CYP1A2 inhibitor

**Cytochrome P450 1A2
inhibitor:** SVM model
built on 9145 molecules
(training set)
and tested on 3000 No
molecules (test set)
10-fold CV: ACC=0.83 /
AUC=0.90
External: ACC=0.84 /
AUC=0.91

CYP2C19 inhibitor

**Cytochrome P450
2C19 inhibitor:** SVM
model built on 9272
molecules (training set)
and tested on 3000 No
molecules (test set)
10-fold CV: ACC=0.80 /
AUC=0.86
External: ACC=0.80 /
AUC=0.87

CYP2C9 inhibitor

**Cytochrome P450 2C9
inhibitor:** SVM model
built on 5940 molecules
(training set)
and tested on 2075 No
molecules (test set)
10-fold CV: ACC=0.78 /
AUC=0.85
External: ACC=0.71 /
AUC=0.81

CYP2D6 inhibitor

**Cytochrome P450 2D6
inhibitor:** SVM model
built on 3664 molecules
(training set)
and tested on 1068 No
molecules (test set)
10-fold CV: ACC=0.79 /
AUC=0.85
External: ACC=0.81 /
AUC=0.87

CYP3A4 inhibitor

**Cytochrome P450 3A4
inhibitor:** SVM model
built on 7518 molecules
(training set)
and tested on 2579 No
molecules (test set)
10-fold CV: ACC=0.77 /
AUC=0.85
External: ACC=0.78 /
AUC=0.86

Log K_p (skin
permeation) -7.16 cm/s

Skin permeation:
QSPR model

[implemented from Potts RO and Guy RH. 1992 Pharm. Res.](#)

Druglikeness

Lipinski ?

Lipinski (Pfizer) filter:

[implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev.](#)
[MW < 500](#)
[MLOGP < 4.15](#)
[N or O < 10](#)
[NH or OH < 5](#)

Yes; 0 violation

Ghose ?

Ghose filter:

[implemented from Ghose AK. et al. 1999 J. Comb. Chem.](#)
[160 < MW < 480](#)
[-0.4 < WLOGP < 5.6](#)
[40 < MR < 130](#)
[20 < atoms < 70](#)

Yes

Veber ?

Veber (GSK) filter:

[implemented from Veber DF. et al. 2002 J. Med. Chem.](#)
[Rotatable bonds < 10](#)
[TPSA < 140](#)

Yes

Egan ?

Egan (Pharmacia) filter:

[implemented from Egan WJ. et al. 2000 J. Med. Chem.](#)
[WLOGP < 5.88](#)
[TPSA < 131.6](#)

Yes

Muegge ?

Muegge (Bayer) filter:

[implemented from Muegge I. et al. 2001 J. Med. Chem.](#)
[200 < MW < 600](#)
[-2 < XLOGP < 5](#)
[TPSA < 150](#)
[Num. rings < 7](#)
[Num. carbon > 4](#)
[Num. heteroatoms > 1](#)
[Num. rotatable bonds < 15](#)
[H-bond acc. < 10](#)
[H-bond don. < 5](#)

Yes

Bioavailability Score ?

Abbott Bioavailability

Score: Probability of F
[> 10% in rat](#)
[implemented from Martin YC. 2005 J. Med. Chem.](#)

0.55

Medicinal Chemistry

PAINS ?

0 alert

Pan Assay Interference Structures:

[implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.](#)

Brenk

Structural Alert:

[implemented from Brenk R. et al. 2008 ChemMedChem](#) 0 alert

Leadlikeness

Leadlikeness:

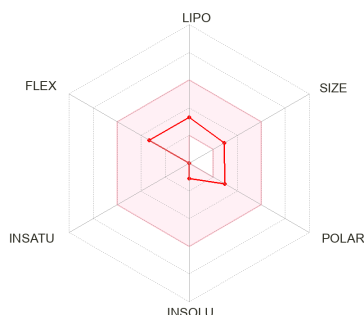
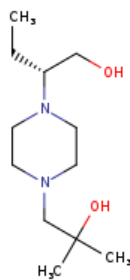
[implemented from Teague SJ. 1999 Angew. Chem. Int. Ed.](#) No; 2 violations: MW<250, Rotors>7
[250 < MW < 350](#)
[XLOGP < 3.5](#)
[Num. rotatable bonds < 7](#)

Synthetic accessibility

Synthetic accessibility

score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penalties, trained on 12'782'590 molecules and tested on 40 external molecules ($r^2 = 0.94$) 2.61

Molecule 7



SMILES CC[C@@H](N1CCN(CC1)CC(O)(C)C)CO

Physicochemical Properties

Formula C12H26N2O2
 Molecular weight 230.35 g/mol
 Num. heavy atoms 16
 Num. arom. heavy atoms 0
 Fraction Csp3 1.00
 Num. rotatable bonds 5
 Num. H-bond acceptors 4
 Num. H-bond donors 2
 Molar Refractivity 73.67
 TPSA 46.94 Å²

Topological Polar

Surface Area:
[Calculated from](#)

Log *S* (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.

Water Solubility

-1.11

Solubility Class

1.77e+01 mg/ml ; 7.68e-02 mol/l

Solubility class: Log *S* scale
 Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Log *S* (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.

-0.83

Solubility Class

3.43e+01 mg/ml ; 1.49e-01 mol/l
 Very soluble

Solubility class: Log *S* scale
 Insoluble < -10 < Poorly < -6 < Moderately < -4

Ertl P. et al. 2000 J. Med. Chem.		< Soluble < -2 Very < 0 < Highly
Log $P_{o/w}$ (iLOGP)	Lipophilicity	Log S (SILICOS-IT)
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.55	SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com
Log $P_{o/w}$ (XLOGP3)		Solubility Class
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.	0.28	2.34e+01 mg/ml ; 1.02e-01 mol/l Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly
Log $P_{o/w}$ (WLOGP)		Pharmacokinetics
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	-0.62	GI absorption
Log $P_{o/w}$ (MLOGP)		Gastrointestinal absorption: according to the white of the BOILED-Egg
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	0.36	BBB permeant
Log $P_{o/w}$ (SILICOS-IT)		BBB permeation: according to the yolk of the BOILED-Egg
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	0.72	P-gp substrate
Consensus Log $P_{o/w}$		P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94
Consensus Log $P_{o/w}$: Average of all five predictions	0.66	CYP1A2 inhibitor
		Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91
		CYP2C19 inhibitor
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87

CYP2C9 inhibitor ⓘ

Cytochrome P450 2C9**inhibitor:** SVM model

built on 5940 molecules

(training set)

and tested on 2075 No

molecules (test set)

10-fold CV: ACC=0.78 /

AUC=0.85

External: ACC=0.71 /

AUC=0.81

CYP2D6 inhibitor ⓘ

Cytochrome P450 2D6**inhibitor:** SVM model

built on 3664 molecules

(training set)

and tested on 1068 No

molecules (test set)

10-fold CV: ACC=0.79 /

AUC=0.85

External: ACC=0.81 /

AUC=0.87

CYP3A4 inhibitor ⓘ

Cytochrome P450 3A4**inhibitor:** SVM model

built on 7518 molecules

(training set)

and tested on 2579 No

molecules (test set)

10-fold CV: ACC=0.77 /

AUC=0.85

External: ACC=0.78 /

AUC=0.86

Log K_p (skin
permeation) ⓘ**Skin permeation:**

QSPR model

-7.51 cm/s

implemented from

Potts RO and Guy RH.

1992 Pharm. Res.

Druglikeness

Lipinski ⓘ

Lipinski (Pfizer) filter:

implemented from

Lipinski CA. et al. 2001

Adv. Drug Deliv. Rev. Yes; 0 violation

MW < 500

MLOGP < 4.15

N or O < 10

NH or OH < 5

Ghose ⓘ

Ghose filter:

implemented from

Ghose AK. et al. 1999 J.

Comb. Chem.

No; 1 violation: WLOGP < -0.4

160 < MW < 480

-0.4 < WLOGP < 5.6

40 < MR < 130

20 < atoms < 70

Veber ⓘ

Yes

Veber (GSK) filter:

implemented from

Veber DE. et al. 2002 J.

Med. Chem.

[Rotatable bonds < 10](#)
[TPSA < 140](#)

Egan

Egan (Pharmacia)

filter: [implemented](#)

[from](#)

[Egan W.J. et al. 2000 J.](#) Yes

[Med. Chem.](#)

[WLOGP < 5.88](#)

[TPSA < 131.6](#)

Muegge

Muegge (Bayer) filter:

[implemented from](#)

[Muegge I. et al. 2001 J.](#)

[Med. Chem.](#)

[200 < MW < 600](#)

[-2 < XLOGP < 5](#)

[TPSA < 150](#) Yes

[Num. rings < 7](#)

[Num. carbon > 4](#)

[Num. heteroatoms > 1](#)

[Num. rotatable bonds <](#)

[15](#)

[H-bond acc. < 10](#)

[H-bond don. < 5](#)

Bioavailability Score

Abbott Bioavailability

Score: [Probability of F](#)

[> 10% in rat](#) 0.55

[implemented from](#)

[Martin Y.C. 2005 J.](#)

[Med. Chem.](#)

Medicinal Chemistry

PAINS

Pan Assay Interference

Structures:

[implemented from](#) 0 alert

[Baell JB. & Holloway](#)

[GA. 2010 J. Med.](#)

[Chem.](#)

Brenk

Structural Alert:

[implemented from](#) 0 alert

[Brenk R. et al. 2008](#)

[ChemMedChem](#)

Leadlikeness

Leadlikeness:

[implemented from](#)

[Teague S.J. 1999 Angew.](#)

[Chem. Int. Ed.](#) No; 1 violation: MW<250

[250 < MW < 350](#)

[XLOGP < 3.5](#)

[Num. rotatable bonds <](#)

[7](#)

Synthetic accessibility 2.36

Synthetic accessibility

score: [from 1 \(very](#)

[easy\) to 10 \(very](#)

[difficult\)](#)

[based on 1024](#)

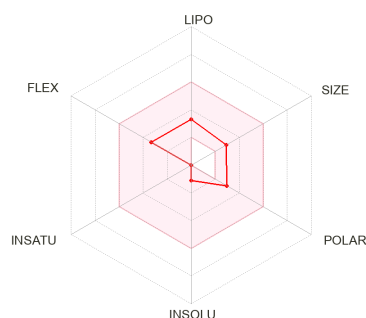
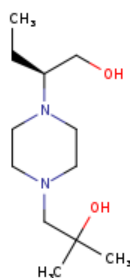
[fragmental contributions](#)

[\(FP2\) modulated by size](#)

[and complexity penalties.](#)

trained on 12'782'590
molecules and tested on
40 external molecules
($r^2 = 0.94$)

Molecule 8



SMILES
S CC[C@H](N1CCN(CC1)CC(O)(C)C)CO

Physicochemical Properties

Formula	C12H26N2O2
Molecular weight	230.35 g/mol
Num. heavy atoms	16
Num. arom. heavy atoms	0
Fraction Csp3	1.00
Num. rotatable bonds	5
Num. H-bond acceptors	4
Num. H-bond donors	2
Molar Refractivity	73.67
TPSA	

Topological Polar Surface Area: 46.94 Å²
Calculated from
[Ertl P. et al. 2000 J. Med. Chem.](#)

Lipophilicity

Log $P_{o/w}$ (iLOGP) 2.56
iLOGP: in-house physics-based method implemented from
[Daina A et al. 2014 J. Chem. Inf. Model.](#)

Log $P_{o/w}$ (XLOGP3) 0.28
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.

Log $P_{o/w}$ (WLOGP) -0.62
WLOGP: Atomistic method implemented from
[Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.](#)

Log S (ESOL)

ESOL: Topological method implemented from
[Delaney JS. 2004 J. Chem. Inf. Model.](#)

Solubility Class 1.77e+01 mg/ml ; 7.68e-02 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Log S (Ali)

Ali: Topological method implemented from
[Ali J. et al. 2012 J. Chem. Inf. Model.](#)

Solubility Class 3.43e+01 mg/ml ; 1.49e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Log S (SILICOS-IT)

SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT,
<http://www.silicos-it.com>

Solubility Class 2.34e+01 mg/ml ; 1.02e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Water Solubility

-1.11

1.77e+01 mg/ml ; 7.68e-02 mol/l

Very soluble

-0.83

3.43e+01 mg/ml ; 1.49e-01 mol/l

Very soluble

-0.99

2.34e+01 mg/ml ; 1.02e-01 mol/l


Soluble

Pharmacokinetics


GI absorption

Gastrointestinal absorption: according to the white of the BOILED-Egg


High

Log $P_{o/w}$ (MLOGP) **MLOGP: Topological method implemented from**[Moriguchi I. et al. 1992 Chem. Pharm. Bull.](#)[Moriguchi I. et al. 1994 Chem. Pharm. Bull.](#)[Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.](#)


0.36

Log $P_{o/w}$ (SILICOS-IT) **SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>**


0.72

Consensus Log $P_{o/w}$ **Consensus Log $P_{o/w}$: Average of all five predictions**


0.66

BBB permeant **BBB permeation:** [according to the yolk of the BOILED-Egg](#)


No

P-gp substrate **P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94**


Yes

CYP1A2 inhibitor **Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91**


No

CYP2C19 inhibitor **Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87**


No

CYP2C9 inhibitor **Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set). 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81**

No


CYP2D6 inhibitor **Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set). 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87**

No

CYP3A4 inhibitor **Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set)**

No

and tested on 2579
 molecules (test set)
 10-fold CV: ACC=0.77 /
 AUC=0.85
 External: ACC=0.78 /
 AUC=0.86

Log K_p (skin
 permeation) 

Skin permeation:

[QSPR model](#) -7.51 cm/s
 implemented from
[Potts RO and Guy RH.](#)
[1992 Pharm. Res.](#)

Druglikeness

Lipinski 

Lipinski (Pfizer) filter:

implemented from
[Lipinski CA. et al. 2001](#)
[Adv. Drug Deliv. Rev.](#) Yes; 0 violation
 MW < 500
 MLOGP < 4.15
 N or O < 10
 NH or OH < 5

Ghose 

Ghose filter:

implemented from
[Ghose AK. et al. 1999 J.](#)
[Comb. Chem.](#) No; 1 violation: WLOGP<-0.4
 160 < MW < 480
 -0.4 < WLOGP < 5.6
 40 < MR < 130
 20 < atoms < 70

Veber 


Veber (GSK) filter:

implemented from
[Veber DF. et al. 2002 J.](#) Yes
[Med. Chem.](#)
 Rotatable bonds < 10
 TPSA < 140

Egan 

**Egan (Pharmacia)
 filter:** implemented

from
[Egan WJ. et al. 2000 J.](#) Yes
[Med. Chem.](#)
 WLOGP < 5.88
 TPSA < 131.6

Muegge 

Muegge (Bayer) filter:

implemented from
[Muegge I. et al. 2001 J.](#)
[Med. Chem.](#)
 200 < MW < 600
 -2 < XLOGP < 5
 TPSA < 150 Yes
 Num. rings < 7
 Num. carbon > 4
 Num. heteroatoms > 1
 Num. rotatable bonds <
 15
 H-bond acc. < 10
 H-bond don. < 5

Bioavailability Score

Abbott Bioavailability:**Score:** Probability of F

> 10% in rat 0.55

implemented from

Martin YC. 2005 J.

Med. Chem.

Medicinal Chemistry

PAINS

Pan Assay Interference**Structures:**

implemented from 0 alert

Baell JB. & Holloway

GA. 2010 J. Med.

Chem.

Brenk

Structural Alert:

implemented from 0 alert

Brenk R. et al. 2008

ChemMedChem

Leadlikeness

Leadlikeness:

implemented from

Teague SJ. 1999 Angew.

Chem. Int. Ed.

No; 1 violation: MW<250

250 < MW < 350

XLOGP < 3.5

Num. rotatable bonds <

7

Synthetic accessibility

Synthetic accessibility**score:** from 1 (very

easy) to 10 (very

difficult)

based on 1024

fragmental contributions 2.36

(FP2) modulated by size

and complexity penalties.

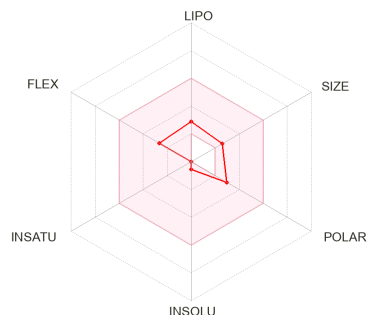
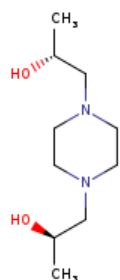
trained on 12'782'590

molecules and tested on

40 external molecules

(r² = 0.94)

Molecule 9



Log S (ESOL)

ESOL: Topological method implemented from

Delaney JS. 2004 J. Chem. Inf. Model.

Water Solubility

-0.56

Solubility

5.58e+01 mg/ml ; 2.76e-01 mol/l

Class

Solubility class: Log S scale

Insoluble < -10 < Poorly

< -6 < Moderately < -4

< Soluble < -2 Very < 0

< Highly

SMILES C[C@H](CN1CCN(CC1)C[C@H](O)C)O

Physicochemical Properties


Formula C10H22N2O2

Molecular weight 202.29 g/mol


Num. heavy atoms 14

Num. arom. heavy atoms	0	Log <i>S</i> (Ali)	
Fraction Csp3	1.00	Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-0.09
Num. rotatable bonds	4		
Num. H-bond acceptors	4		
Num. H-bond donors	2		
Molar Refractivity	64.02	Solubility	1.64e+02 mg/ml ; 8.11e-01 mol/l
TPSA		Class	
Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	46.94 Å ²	Solubility class: Log <i>S</i> scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Very soluble
	Lipophilicity		
Log <i>P</i> _{o/w} (iLOGP)		Log <i>S</i> (SILICOS-IT)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.60	SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-0.20
Log <i>P</i> _{o/w} (XLOGP3)		Solubility	1.28e+02 mg/ml ; 6.32e-01 mol/l
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.	-0.43	Class	
Log <i>P</i> _{o/w} (WLOGP)		Solubility class: Log <i>S</i> scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	-1.40		
Log <i>P</i> _{o/w} (MLOGP)			Pharmacokinetics
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	-0.21	GI absorption	
Log <i>P</i> _{o/w} (SILICOS-IT)		Gastrointestinal absorption: according to the white of the BOILED-Egg	Low
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	0.12	BBB permeant	
Consensus Log <i>P</i> _{o/w}		BBB permeation: according to the yolk of the BOILED-Egg	No
Consensus Log <i>P</i>_{o/w}: Average of all five predictions	0.14	P-gp substrate	
		P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
		CYP1A2 inhibitor	No
		Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.83 / AUC=0.90	


[External: ACC=0.84 / AUC=0.91](#)

CYP2C19 inhibitor 


Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) No
 10-fold CV: ACC=0.80 / AUC=0.86
 External: ACC=0.80 / AUC=0.87

CYP2C9 inhibitor 


Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) No
 10-fold CV: ACC=0.78 / AUC=0.85
 External: ACC=0.71 / AUC=0.81

CYP2D6 inhibitor 

Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) No
 10-fold CV: ACC=0.79 / AUC=0.85
 External: ACC=0.81 / AUC=0.87

CYP3A4 inhibitor 

Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) No
 10-fold CV: ACC=0.77 / AUC=0.85
 External: ACC=0.78 / AUC=0.86

Log K_p (skin permeation) 

Skin permeation: QSPR model implemented from Potts RO and Guy RH. 1992 Pharm. Res. -7.84 cm/s

Druglikeness

Lipinski 

Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. Yes; 0 violation
 MW < 500
 MLOGP < 4.15
 N or O < 10
 NH or OH < 5

Ghose **Ghose filter:**

implemented from

[Ghose AK. et al. 1999 J.](#)[Comb. Chem.](#)[160 < MW < 480](#)[-0.4 < WLOGP < 5.6](#)[40 < MR < 130](#)[20 < atoms < 70](#)

No; 1 violation: WLOGP<-0.4

Veber **Veber (GSK) filter:**

implemented from

[Veber DF. et al. 2002 J.](#)[Med. Chem.](#)[Rotatable bonds < 10](#)[TPSA < 140](#)


Yes

Egan **Egan (Pharmacia)****filter:** implemented

from

[Egan WJ. et al. 2000 J.](#)[Med. Chem.](#)[WLOGP < 5.88](#)[TPSA < 131.6](#)


Yes

Muegge **Muegge (Bayer) filter:**

implemented from

[Muegge I. et al. 2001 J.](#)[Med. Chem.](#)[200 < MW < 600](#)[-2 < XLOGP < 5](#)[TPSA < 150](#)[Num. rings < 7](#)[Num. carbon > 4](#)[Num. heteroatoms > 1](#)[Num. rotatable bonds <](#)[15](#)[H-bond acc. < 10](#)[H-bond don. < 5](#)

Yes

Bioavailability Score **Abbott Bioavailability****Score:** Probability of F[> 10% in rat](#)

implemented from

[Martin YC. 2005 J.](#)[Med. Chem.](#)

0.55

Medicinal Chemistry

PAINS **Pan Assay Interference****Structures:**

implemented from

[Baell JB. & Holloway.](#)[GA. 2010 J. Med.](#)[Chem.](#)

0 alert

Brenk **Structural Alert:**

implemented from

[Brenk R. et al. 2008](#)[ChemMedChem](#)

0 alert

Leadlikeness 

No; 1 violation: MW<250

Leadlikeness:

implemented from

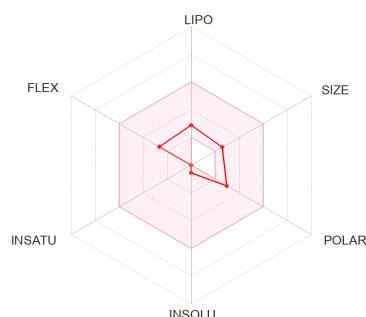
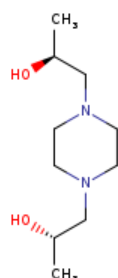
Teague SJ. 1999 Angew.
Chem. Int. Ed.
250 < MW < 350
XLOGP < 3.5
Num. rotatable bonds <
7

Synthetic accessibility

Synthetic accessibility

score: from 1 (very
easy) to 10 (very
difficult)
based on 1024
fragmental contributions 2.44
(FP2) modulated by size
and complexity penalties,
trained on 12'782'590
molecules and tested on
40 external molecules
($r^2 = 0.94$)

Molecule 10



Log *S* (ESOL)

ESOL: Topological method implemented from
Delaney JS. 2004 J. Chem. Inf. Model.

Water Solubility

-0.56

Solubility Class

5.58e+01 mg/ml ; 2.76e-01 mol/l

Solubility class: Log *S* scale
Insoluble < -10 < Poorly
< -6 < Moderately < -4
< Soluble < -2 Very < 0
< Highly

Very soluble

SMILES C[C@@H](CN1CCN(CC1)C[C@@H](O)C)O

Physicochemical Properties

Formula C10H22N2O2
Molecular weight 202.29 g/mol
Num. heavy atoms 14
Num. arom. heavy atoms 0
Fraction Csp3 1.00
Num. rotatable bonds 4
Num. H-bond acceptors 4
Num. H-bond donors 2
Molar Refractivity 64.02
TPSA

Topological Polar Surface Area:
Calculated from
Ertl P. et al. 2000 J. Med. Chem.

46.94 Å²

Log *S* (Ali)

Ali: Topological method implemented from
Ali J. et al. 2012 J. Chem. Inf. Model.

-0.09

Solubility Class

1.64e+02 mg/ml ; 8.11e-01 mol/l

Solubility class: Log *S* scale
Insoluble < -10 < Poorly
< -6 < Moderately < -4
< Soluble < -2 Very < 0
< Highly

Very soluble

Lipophilicity

Log *P*_{o/w} (iLOGP)

iLOGP: in-house physics-based method implemented from
Daina A et al. 2014 J. Chem. Inf. Model.

2.25

Log *P*_{o/w} (XLOGP3)

XLOGP3: Atomistic and knowledge-based

-0.43

Log *S* (SILICOS-IT)

SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>

-0.20

Solubility

1.28e+02 mg/ml ; 6.32e-01 mol/l

[method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.](#)

Log $P_{o/w}$ (WLOGP) [?]

WLOGP: Atomistic method implemented from

[Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.](#)

-1.40

Log $P_{o/w}$ (MLOGP) [?]

MLOGP: Topological method implemented from

[Moriguchi I. et al. 1992 Chem. Pharm. Bull.](#)

[Moriguchi I. et al. 1994 Chem. Pharm. Bull.](#)

[Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.](#)

-0.21

Log $P_{o/w}$ (SILICOS-IT) [?]

SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>

0.12

Consensus Log $P_{o/w}$ [?]

Consensus Log $P_{o/w}$: Average of all five predictions

0.07

Class [?]

Solubility class: Log S scale

[Insoluble < -10 < Poorly Soluble < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly](#)

Pharmacokinetics

GI absorption [?]

Gastrointestinal absorption: according to the white of the BOILED-Egg Low

BBB permeant [?]

BBB permeation: according to the yolk of the BOILED-Egg No

P-gp substrate [?]

P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94 No

CYP1A2 inhibitor [?]


Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91 No

CYP2C19 inhibitor [?]

Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87 No

CYP2C9 inhibitor [?]

Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set). 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81 No

CYP2D6 inhibitor **Cytochrome P450 2D6****inhibitor:** [SVM model](#)[built on 3664 molecules](#)[\(training set\)](#)


and tested on 1068 No

[molecules \(test set\)](#)

10-fold CV: ACC=0.79 /

[AUC=0.85](#)

External: ACC=0.81 /

[AUC=0.87](#)CYP3A4 inhibitor **Cytochrome P450 3A4****inhibitor:** [SVM model](#)[built on 7518 molecules](#)[\(training set\)](#)


and tested on 2579 No

[molecules \(test set\)](#)

10-fold CV: ACC=0.77 /

[AUC=0.85](#)

External: ACC=0.78 /


[AUC=0.86](#)Log K_p (skin
permeation) **Skin permeation:**[QSPR model](#)

-7.84 cm/s

implemented from

[Potts RO and Guy RH.](#)[1992 Pharm. Res.](#)

Druglikeness

Lipinski **Lipinski (Pfizer) filter:**

implemented from

[Lipinski CA. et al. 2001](#)[Adv. Drug Deliv. Rev.](#)

Yes; 0 violation

[MW < 500](#)[MLOGP < 4.15](#)[N or O < 10](#)[NH or OH < 5](#)Ghose **Ghose filter:**

implemented from

[Ghose AK. et al. 1999 J.](#)[Comb. Chem.](#)

No; 1 violation: WLOGP<-0.4

[160 < MW < 480](#)[-0.4 < WLOGP < 5.6](#)[40 < MR < 130](#)[20 < atoms < 70](#)Veber **Veber (GSK) filter:**

implemented from

[Veber DF. et al. 2002 J.](#)

Yes


[Med. Chem.](#)[Rotatable bonds < 10](#)[TPSA < 140](#)Egan **Egan (Pharmacia)****filter:** implemented

from


[Egan WJ. et al. 2000 J.](#)

Yes

[Med. Chem.](#)[WLOGP < 5.88](#)[TPSA < 131.6](#)

Muegge **Muegge (Bayer) filter:**

implemented from
[Muegge I. et al. 2001 J. Med. Chem.](#)
 $200 < MW < 600$
 $-2 < XLOGP < 5$
 $TPSA < 150$ Yes
 $Num. rings < 7$
 $Num. carbon > 4$
 $Num. heteroatoms > 1$
 $Num. rotatable bonds < 15$
 $H-bond acc. < 10$
 $H-bond don. < 5$

Bioavailability Score **Abbott Bioavailability**

Score: Probability of F
 $> 10\%$ in rat 0.55
 implemented from
[Martin YC. 2005 J. Med. Chem.](#)

Medicinal Chemistry

PAINS **Pan Assay Interference**


Structures:
 implemented from 0 alert
[Baell JB. & Holloway GA. 2010 J. Med. Chem.](#)

Brenk **Structural Alert:**

implemented from 0 alert
[Brenk R. et al. 2008 ChemMedChem](#)

Leadlikeness **Leadlikeness:**

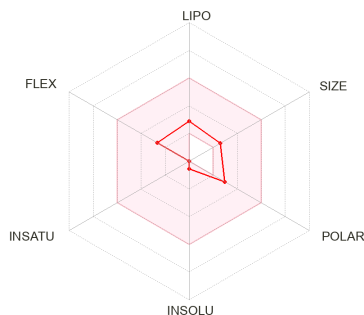
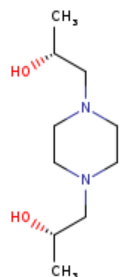
implemented from
[Teague SJ. 1999 Angew. Chem. Int. Ed.](#) No; 1 violation: MW<250
 $250 < MW < 350$
 $XLOGP < 3.5$
 $Num. rotatable bonds < 7$

Synthetic accessibility **Synthetic accessibility**

score: from 1 (very easy) to 10 (very difficult)
 based on 1024
[fragmental contributions \(FP2\) modulated by size and complexity penalties, trained on 12'782'590 molecules and tested on 40 external molecules](#) 2.44
 $(r^2 = 0.94)$

Molecule 11

Water Solubility 



SMILES C[C@H](CN1CCN(CC1)C[C@@H](O)C)O

Physicochemical Properties

Formula	C10H22N2O2
Molecular weight	202.29 g/mol
Num. heavy atoms	14
Num. arom. heavy atoms	0
Fraction Csp3	1.00
Num. rotatable bonds	4
Num. H-bond acceptors	4
Num. H-bond donors	2
Molar Refractivity	64.02
TPSA	

Topological Polar Surface Area:
Calculated from
Ertl P. et al. 2000 J. Med. Chem.

46.94 Å²

Lipophilicity

Log $P_{o/w}$ (iLOGP)

iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.

2.58

Log $P_{o/w}$ (XLOGP3)

XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry

-0.43

Log $P_{o/w}$ (WLOGP)

WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.

-1.40

Log $P_{o/w}$ (MLOGP)

MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull.

-0.21

Log S (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.

-0.56

Solubility Class

5.58e+01 mg/ml ; 2.76e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Very soluble

Log S (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.

-0.09

Solubility Class

1.64e+02 mg/ml ; 8.11e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Very soluble

Log S (SILICOS-IT)

SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>

-0.20

Solubility Class

1.28e+02 mg/ml ; 6.32e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Soluble

Pharmacokinetics

GI absorption

Gastrointestinal absorption: according to the white of the BOILED-Egg

Low

BBB permeant

BBB permeation: according to the yolk of the BOILED-Egg

No

P-gp substrate

P-glycoprotein substrate: SVM model built on 1033 molecules

No

[Lipinski PA. et al. 2001
Adv. Drug. Deliv. Rev.](#)
Log $P_{o/w}$ (SILICOS-IT)

SILICOS-IT: Hybrid
fragmental/topological
method calculated by
FILTER-IT program,
version 1.0.2, courtesy
of SILICOS-IT,
[http://www.silicos-
it.com](http://www.silicos-
it.com)

0.12

Consensus Log $P_{o/w}$

Consensus Log $P_{o/w}$:
Average of all five
predictions

0.13

(training set)
and tested on 415
molecules (test set)
10-fold CV: ACC=0.72 /
AUC=0.77
External: ACC=0.88 /
AUC=0.94
CYP1A2 inhibitor

**Cytochrome P450 1A2
inhibitor:** SVM model
built on 9145 molecules
(training set)
and tested on 3000
molecules (test set) No
10-fold CV: ACC=0.83 /
AUC=0.90
External: ACC=0.84 /
AUC=0.91

CYP2C19 inhibitor

**Cytochrome P450
2C19 inhibitor:** SVM
model built on 9272
molecules (training set) No
and tested on 3000
molecules (test set)
10-fold CV: ACC=0.80 /
AUC=0.86
External: ACC=0.80 /
AUC=0.87

CYP2C9 inhibitor

**Cytochrome P450 2C9
inhibitor:** SVM model
built on 5940 molecules
(training set) No
and tested on 2075
molecules (test set)
10-fold CV: ACC=0.78 /
AUC=0.85
External: ACC=0.71 /
AUC=0.81

CYP2D6 inhibitor

**Cytochrome P450 2D6
inhibitor:** SVM model
built on 3664 molecules
(training set) No
and tested on 1068
molecules (test set)
10-fold CV: ACC=0.79 /
AUC=0.85
External: ACC=0.81 /
AUC=0.87

CYP3A4 inhibitor

**Cytochrome P450 3A4
inhibitor:** SVM model
built on 7518 molecules
(training set) No
and tested on 2579
molecules (test set)
10-fold CV: ACC=0.77 /
AUC=0.85
External: ACC=0.78 /
AUC=0.86

Log K_p (skin
permeation) -7.84 cm/s

Skin permeation:
QSPR model

[implemented from Potts RO and Guy RH. 1992 Pharm. Res.](#)

Druglikeness

Lipinski [?]

Lipinski (Pfizer) filter:

[implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev.](#)
[MW < 500](#)
[MLOGP < 4.15](#)
[N or O < 10](#)
[NH or OH < 5](#)

Yes; 0 violation

Ghose [?]

Ghose filter:

[implemented from Ghose AK. et al. 1999 J. Comb. Chem.](#)
[160 < MW < 480](#)
[-0.4 < WLOGP < 5.6](#)
[40 < MR < 130](#)
[20 < atoms < 70](#)

No; 1 violation: WLOGP < -0.4

Veber [?]

Veber (GSK) filter:

[implemented from Veber DF. et al. 2002 J. Med. Chem.](#)
[Rotatable bonds < 10](#)
[TPSA < 140](#)

Yes

Egan [?]

Egan (Pharmacia) filter:

[implemented from Egan WJ. et al. 2000 J. Med. Chem.](#)
[WLOGP < 5.88](#)
[TPSA < 131.6](#)

Yes

Muegge [?]

Muegge (Bayer) filter:

[implemented from Muegge I. et al. 2001 J. Med. Chem.](#)
[200 < MW < 600](#)
[-2 < XLOGP < 5](#)
[TPSA < 150](#)
[Num. rings < 7](#)
[Num. carbon > 4](#)
[Num. heteroatoms > 1](#)
[Num. rotatable bonds < 15](#)
[H-bond acc. < 10](#)
[H-bond don. < 5](#)

Yes

Bioavailability Score [?]

Abbott Bioavailability

Score: Probability of F
[> 10% in rat](#)
[implemented from Martin YC. 2005 J. Med. Chem.](#)

0.55

Medicinal Chemistry

PAINS [?]

0 alert

Pan Assay Interference Structures:

[implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.](#)

Brenk

Structural Alert:

[implemented from Brenk R. et al. 2008 ChemMedChem](#) 0 alert

Leadlikeness

Leadlikeness:

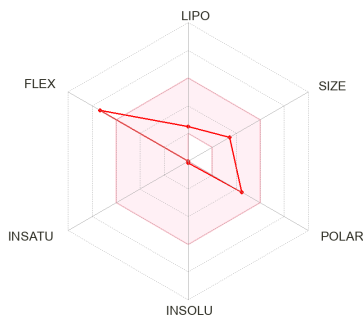
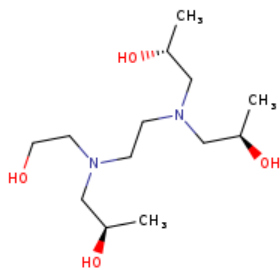
[implemented from Teague SJ. 1999 Angew. Chem. Int. Ed.](#) No; 1 violation: MW<250
[250 < MW < 350](#)
[XLOGP < 3.5](#)
[Num. rotatable bonds < 7](#)

Synthetic accessibility

Synthetic accessibility

score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penalties, trained on 12'782'590 molecules and tested on 40 external molecules ($r^2 = 0.94$) 2.44

Molecule 12



SMILES OCCN(C[C@H](O)C)CCN(C[C@H](O)C)C[C@H](O)C

Physicochemical Properties

Formula	C13H30N2O4
Molecular weight	278.39 g/mol
Num. heavy atoms	19
Num. arom. heavy atoms	0
Fraction Csp3	1.00
Num. rotatable bonds	11
Num. H-bond acceptors	6
Num. H-bond donors	4
Molar Refractivity	75.04
TPSA	87.40 Å ²

Topological Polar

Surface Area:
[Calculated from](#)

Log *S* (ESOL)

ESOL: [Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.](#)

Water Solubility

-0.12

Solubility Class

2.10e+02 mg/ml ; 7.55e-01 mol/l

Solubility class: Log *S* scale
 Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Log *S* (Ali)

Ali: [Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.](#)

-0.20

Solubility Class

1.74e+02 mg/ml ; 6.26e-01 mol/l
 Very soluble

Solubility class: Log *S* scale
 Insoluble < -10 < Poorly < -6 < Moderately < -4

Ertl P. et al. 2000 J. Med. Chem.		< Soluble < -2 Very < 0 < Highly
Log $P_{o/w}$ (iLOGP)	Lipophilicity	Log S (SILICOS-IT)
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.82	SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com
Log $P_{o/w}$ (XLOGP3)		Solubility Class
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.	-1.14	1.13e+02 mg/ml ; 4.06e-01 mol/l Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly
Log $P_{o/w}$ (WLOGP)		Pharmacokinetics
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	-1.27	GI absorption
Log $P_{o/w}$ (MLOGP)		Gastrointestinal absorption: according to the white of the BOILED-Egg
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	-0.62	BBB permeant
Log $P_{o/w}$ (SILICOS-IT)		BBB permeation: according to the yolk of the BOILED-Egg
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-0.16	P-gp substrate
Consensus Log $P_{o/w}$		P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94
Consensus Log $P_{o/w}$: Average of all five predictions	-0.07	CYP1A2 inhibitor
		Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91
		CYP2C19 inhibitor
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87

CYP2C9 inhibitor ⓘ

Cytochrome P450 2C9**inhibitor:** SVM model

built on 5940 molecules

(training set)

and tested on 2075 No

molecules (test set)

10-fold CV: ACC=0.78 /

AUC=0.85

External: ACC=0.71 /

AUC=0.81

CYP2D6 inhibitor ⓘ

Cytochrome P450 2D6**inhibitor:** SVM model

built on 3664 molecules

(training set)

and tested on 1068 No

molecules (test set)

10-fold CV: ACC=0.79 /

AUC=0.85

External: ACC=0.81 /

AUC=0.87

CYP3A4 inhibitor ⓘ

Cytochrome P450 3A4**inhibitor:** SVM model

built on 7518 molecules

(training set)

and tested on 2579 No

molecules (test set)

10-fold CV: ACC=0.77 /

AUC=0.85

External: ACC=0.78 /

AUC=0.86

Log K_p (skin
permeation) ⓘ**Skin permeation:**

QSPR model

-8.81 cm/s

implemented from

Potts RO and Guy RH.

1992 Pharm. Res.

Druglikeness

Lipinski ⓘ

Lipinski (Pfizer) filter:

implemented from

Lipinski CA. et al. 2001

Adv. Drug Deliv. Rev. Yes; 0 violation

MW < 500

MLOGP < 4.15

N or O < 10

NH or OH < 5

Ghose ⓘ

Ghose filter:

implemented from

Ghose AK. et al. 1999 J.

Comb. Chem.

No; 1 violation: WLOGP<-0.4

160 < MW < 480

-0.4 < WLOGP < 5.6

40 < MR < 130

20 < atoms < 70

Veber ⓘ

No; 1 violation: Rotors>10

Veber (GSK) filter:

implemented from

Veber DE. et al. 2002 J.

Med. Chem.


[Rotatable bonds < 10](#)
[TPSA < 140](#)

Egan 

Egan (Pharmacia)

filter: [implemented](#)


[from](#)
[Egan W.J. et al. 2000 J. Med. Chem.](#) Yes
[WLOGP < 5.88](#)
[TPSA < 131.6](#)

Muegge 

Muegge (Bayer) filter:

[implemented from](#)

[Muegge I. et al. 2001 J. Med. Chem.](#) Yes
[200 < MW < 600](#)
[-2 < XLOGP < 5](#)
[TPSA < 150](#)
[Num. rings < 7](#)
[Num. carbon > 4](#)
[Num. heteroatoms > 1](#)
[Num. rotatable bonds < 15](#)
[H-bond acc. < 10](#)
[H-bond don. < 5](#)

Bioavailability Score 

Abbott Bioavailability

Score: [Probability of F > 10% in rat](#) 0.55
[implemented from](#)
[Martin Y.C. 2005 J. Med. Chem.](#)

Medicinal Chemistry

PAINS 

Pan Assay Interference

Structures:

[implemented from](#) 0 alert
[Baell JB. & Holloway GA. 2010 J. Med. Chem.](#)

Brenk 


Structural Alert:

[implemented from](#) 0 alert
[Brenk R. et al. 2008 ChemMedChem](#)

Leadlikeness 

Leadlikeness:

[implemented from](#)
[Teague S.J. 1999 Angew. Chem. Int. Ed.](#) No; 1 violation: Rotors>7
[250 < MW < 350](#)
[XLOGP < 3.5](#)
[Num. rotatable bonds < 7](#)

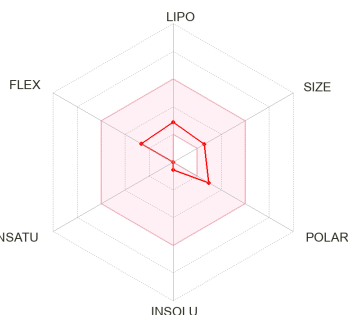
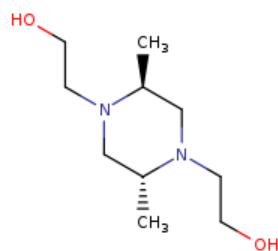
Synthetic accessibility  3.18

Synthetic accessibility

score: [from 1 \(very easy\) to 10 \(very difficult\)](#)
[based on 1024 fragmental contributions \(FP2\) modulated by size and complexity penalties.](#)

trained on 12'782'590
molecules and tested on
40 external molecules
($r^2 = 0.94$)

Molecule 13



SMILES OCCN1C[C@H](C)N(C[C@H]1C)CCO

Physicochemical Properties

Formula	C10H22N2O2
Molecular weight	202.29 g/mol
Num. heavy atoms	14
Num. arom. heavy atoms	0
Fraction Csp3	1.00
Num. rotatable bonds	4
Num. H-bond acceptors	4
Num. H-bond donors	2
Molar Refractivity	64.02
TPSA	

Topological Polar Surface Area:

46.94 Å²
Calculated from
Ertl P. et al. 2000 J.
Med. Chem.

Lipophilicity

Log $P_{o/w}$ (iLOGP)

iLOGP: in-house
physics-based method
implemented from
Daina A et al. 2014 J.
Chem. Inf. Model.

2.11

Log $P_{o/w}$ (XLOGP3)

XLOGP3: Atomistic
and knowledge-based
method calculated by
XLOGP program,
version 3.2.2, courtesy
of CCBG, Shanghai
Institute of Organic
Chemistry.

-0.43

Log $P_{o/w}$ (WLOGP)

WLOGP: Atomistic
method implemented
from
Wildman SA and
Crippen GM. 1999 J.
Chem. Inf. Model.

-1.40

Log S (ESOL)

ESOL: Topological
method implemented
from
Delaney JS. 2004 J.
Chem. Inf. Model.

Water Solubility

-0.56

Solubility
Class

5.58e+01 mg/ml ; 2.76e-01 mol/l

Solubility class: Log S
scale

Insoluble < -10 < Poorly
< -6 < Moderately < -4
< Soluble < -2 Very < 0
< Highly

Very soluble

Log S (Ali)

Ali: Topological method
implemented from
Ali J. et al. 2012 J.
Chem. Inf. Model.

-0.09

Solubility
Class

1.64e+02 mg/ml ; 8.11e-01 mol/l

Solubility class: Log S
scale

Insoluble < -10 < Poorly
< -6 < Moderately < -4
< Soluble < -2 Very < 0
< Highly

Very soluble

Log S (SILICOS-IT)

SILICOS-IT:
Fragmental method
calculated by
FILTER-IT program,
version 1.0.2, courtesy
of SILICOS-IT,
[http://www.silicos-
it.com](http://www.silicos-it.com)

-0.45

Solubility
Class

7.18e+01 mg/ml ; 3.55e-01 mol/l

Solubility class: Log S
scale

Insoluble < -10 < Poorly
< -6 < Moderately < -4
< Soluble < -2 Very < 0
< Highly


Soluble

Pharmacokinetics


GI absorption

**Gastrointestinal
absorption:** according
to the white of the
BOILED-Egg


Low

Log $P_{o/w}$ (MLOGP) **MLOGP: Topological method implemented from**








[Moriguchi I. et al. 1992 Chem. Pharm. Bull.](#) -0.21
[Moriguchi I. et al. 1994 Chem. Pharm. Bull.](#)
[Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.](#)

Log $P_{o/w}$ (SILICOS-IT) **SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>**


-0.11

Consensus Log $P_{o/w}$ **Consensus Log $P_{o/w}$: Average of all five predictions**

-0.01

BBB permeant **BBB permeation:** according to the yolk of the BOILED-Egg NoP-gp substrate **P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94** NoCYP1A2 inhibitor **Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91** NoCYP2C19 inhibitor **Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87** NoCYP2C9 inhibitor **Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set). 10-fold CV: ACC=0.78 / AUC=0.85 External: ACC=0.71 / AUC=0.81** NoCYP2D6 inhibitor **Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set). 10-fold CV: ACC=0.79 / AUC=0.85 External: ACC=0.81 / AUC=0.87** NoCYP3A4 inhibitor  No**Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set).**

and tested on 2579
 molecules (test set)
 10-fold CV: ACC=0.77 /
 AUC=0.85
 External: ACC=0.78 /
 AUC=0.86

Log K_p (skin
 permeation) 

Skin permeation:

[QSPR model](#) -7.84 cm/s
 implemented from
[Potts RO and Guy RH.](#)
[1992 Pharm. Res.](#)

Druglikeness

Lipinski 

Lipinski (Pfizer) filter:

implemented from
[Lipinski CA. et al. 2001](#)
[Adv. Drug Deliv. Rev.](#) Yes; 0 violation
 MW < 500
 MLOGP < 4.15
 N or O < 10
 NH or OH < 5

Ghose 

Ghose filter:

implemented from
[Ghose AK. et al. 1999 J.](#)
[Comb. Chem.](#) No; 1 violation: WLOGP<-0.4
 160 < MW < 480
 -0.4 < WLOGP < 5.6
 40 < MR < 130
 20 < atoms < 70

Veber 


Veber (GSK) filter:

implemented from
[Veber DF. et al. 2002 J.](#) Yes
[Med. Chem.](#)
 Rotatable bonds < 10
 TPSA < 140

Egan 

**Egan (Pharmacia)
 filter:** implemented

from
[Egan WJ. et al. 2000 J.](#) Yes
[Med. Chem.](#)
 WLOGP < 5.88
 TPSA < 131.6

Muegge 

Muegge (Bayer) filter:

implemented from
[Muegge I. et al. 2001 J.](#)
[Med. Chem.](#)
 200 < MW < 600
 -2 < XLOGP < 5
 TPSA < 150 Yes
 Num. rings < 7
 Num. carbon > 4
 Num. heteroatoms > 1
 Num. rotatable bonds <
 15
 H-bond acc. < 10
 H-bond don. < 5

Bioavailability Score

Abbott Bioavailability:

Score: Probability of F
 > 10% in rat 0.55
 implemented from
[Martin YC. 2005 J. Med. Chem.](#)

Medicinal Chemistry

PAINS

Pan Assay Interference

Structures:
 implemented from 0 alert
[Baell JB. & Holloway GA. 2010 J. Med. Chem.](#)

Brenk

Structural Alert:

implemented from 0 alert
[Brenk R. et al. 2008 ChemMedChem](#)

Leadlikeness

Leadlikeness:

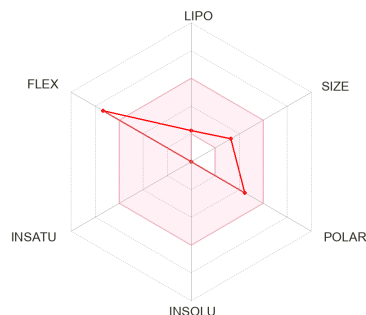
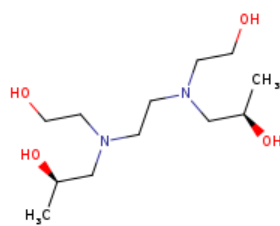
implemented from
[Teague SJ. 1999 Angew. Chem. Int. Ed.](#) No; 1 violation: MW<250
 250 < MW < 350
 XLOGP < 3.5
 Num. rotatable bonds < 7

Synthetic accessibility

Synthetic accessibility

score: from 1 (very easy) to 10 (very difficult)
 based on 1024 fragmental contributions 2.51
 (FP2) modulated by size and complexity penalties,
 trained on 12'782'590 molecules and tested on 40 external molecules
 ($r^2 = 0.94$)

Molecule 14



Log S (ESOL)

ESOL: Topological method implemented from
[Delaney JS. 2004 J. Chem. Inf. Model.](#)

Water Solubility

0.24

Solubility Class

4.55e+02 mg/ml ; 1.72e+00 mol/l

Solubility class: Log S scale

Insoluble < -10 < Poorly
 < -6 < Moderately < -4
 < Soluble < -2 Very < 0
 < Highly


SMILES
 S OCCN(C[C@H](O)C)CCN(C[C@H](O)C)CCO

Physicochemical Properties


Formula C12H28N2O4
 Molecular weight 264.36 g/mol
 Num. heavy atoms 18

Num. arom. heavy atoms	0	Log <i>S</i> (Ali)	
Fraction Csp3	1.00	Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	0.24
Num. rotatable bonds	11		
Num. H-bond acceptors	6		
Num. H-bond donors	4		
Molar Refractivity	70.24	Solubility Class	4.62e+02 mg/ml ; 1.75e+00 mol/l
TPSA		Solubility class: Log <i>S</i> scale	
Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	87.40 Å ²	Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Highly soluble
	Lipophilicity		
Log <i>P</i> _{o/w} (iLOGP)		Log <i>S</i> (SILICOS-IT)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.62	SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-0.37
Log <i>P</i> _{o/w} (XLOGP3)		Solubility Class	1.14e+02 mg/ml ; 4.31e-01 mol/l
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.	-1.57	Solubility class: Log <i>S</i> scale	Soluble
Log <i>P</i> _{o/w} (WLOGP)		Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	-1.66		Pharmacokinetics
Log <i>P</i> _{o/w} (MLOGP)		GI absorption	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	-0.89	Gastrointestinal absorption: according to the white of the BOILED-Egg	High
Log <i>P</i> _{o/w} (SILICOS-IT)		BBB permeant	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-0.41	BBB permeation: according to the yolk of the BOILED-Egg	No
Consensus Log <i>P</i> _{o/w}		P-gp substrate	
Consensus Log <i>P</i>_{o/w}: Average of all five predictions	-0.38	P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
		CYP1A2 inhibitor	No
		Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.83 / AUC=0.90	


[External: ACC=0.84 / AUC=0.91](#)

CYP2C19 inhibitor 


Cytochrome P450 2C19 inhibitor: SVM model built on [9272 molecules \(training set\)](#) and tested on [3000 molecules \(test set\)](#) No
 10-fold CV: ACC=0.80 / AUC=0.86
 External: ACC=0.80 / AUC=0.87

CYP2C9 inhibitor 


Cytochrome P450 2C9 inhibitor: SVM model built on [5940 molecules \(training set\)](#) and tested on [2075 molecules \(test set\)](#) No
 10-fold CV: ACC=0.78 / AUC=0.85
 External: ACC=0.71 / AUC=0.81

CYP2D6 inhibitor 

Cytochrome P450 2D6 inhibitor: SVM model built on [3664 molecules \(training set\)](#) and tested on [1068 molecules \(test set\)](#) No
 10-fold CV: ACC=0.79 / AUC=0.85
 External: ACC=0.81 / AUC=0.87

CYP3A4 inhibitor 

Cytochrome P450 3A4 inhibitor: SVM model built on [7518 molecules \(training set\)](#) and tested on [2579 molecules \(test set\)](#) No
 10-fold CV: ACC=0.77 / AUC=0.85
 External: ACC=0.78 / AUC=0.86

Log K_p (skin permeation) 

Skin permeation: QSPR model implemented from [Potts RO and Guy RH. 1992 Pharm. Res.](#) -9.03 cm/s

Druglikeness

Lipinski 

Lipinski (Pfizer) filter: implemented from [Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev.](#) Yes; 0 violation
 MW < 500
 MLOGP < 4.15
 N or O < 10
 NH or OH < 5

Ghose ?

Ghose filter:

implemented from

[Ghose AK. et al. 1999 J.](#)[Comb. Chem.](#)[160 < MW < 480](#)[-0.4 < WLOGP < 5.6](#)[40 < MR < 130](#)[20 < atoms < 70](#)

No; 1 violation: WLOGP<-0.4

Veber ?

Veber (GSK) filter:

implemented from

[Veber DF. et al. 2002 J.](#)[Med. Chem.](#)[Rotatable bonds < 10](#)[TPSA < 140](#)

No; 1 violation: Rotors>10

Egan ?

Egan (Pharmacia)**filter:** implemented

from

[Egan WJ. et al. 2000 J.](#)[Med. Chem.](#)[WLOGP < 5.88](#)[TPSA < 131.6](#)

Yes

Muegge ?

Muegge (Bayer) filter:

implemented from

[Muegge I. et al. 2001 J.](#)[Med. Chem.](#)[200 < MW < 600](#)[-2 < XLOGP < 5](#)[TPSA < 150](#)[Num. rings < 7](#)[Num. carbon > 4](#)[Num. heteroatoms > 1](#)[Num. rotatable bonds <](#)[15](#)[H-bond acc. < 10](#)[H-bond don. < 5](#)

Yes

Bioavailability Score ?

Abbott Bioavailability**Score:** Probability of F[> 10% in rat](#)

implemented from

[Martin YC. 2005 J.](#)[Med. Chem.](#)

0.55

Medicinal Chemistry

PAINS ?

Pan Assay Interference**Structures:**

implemented from

[Baell JB. & Holloway.](#)[GA. 2010 J. Med.](#)[Chem.](#)

0 alert

Brenk ?

Structural Alert:

implemented from

[Brenk R. et al. 2008](#)[ChemMedChem](#)

0 alert

Leadlikeness ?

No; 1 violation: Rotors>7

Leadlikeness:

implemented from

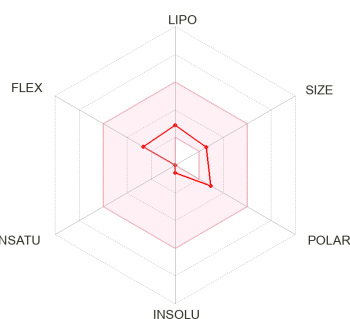
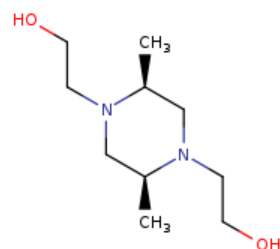
Teague SJ. 1999 Angew.
Chem. Int. Ed.
250 < MW < 350
XLOGP < 3.5
Num. rotatable bonds <
7

Synthetic accessibility [?]

Synthetic accessibility

score: from 1 (very
easy) to 10 (very
difficult)
based on 1024
fragmental contributions 2.84
(FP2) modulated by size
and complexity penalties,
trained on 12'782'590
molecules and tested on
40 external molecules
($r^2 = 0.94$)

Molecule 15



SMILES
S OCCN1C[C@H](C)N(C[C@@H]1C)CCO

Physicochemical Properties

Formula C10H22N2O2
Molecular weight 202.29 g/mol
Num. heavy atoms 14
Num. arom. heavy atoms 0
Fraction Csp3 1.00
Num. rotatable bonds 4
Num. H-bond acceptors 4
Num. H-bond donors 2
Molar Refractivity 64.02
TPSA [?]

**Topological Polar
Surface Area:**
Calculated from
Ertl P. et al. 2000 J.
Med. Chem.

46.94 Å²

Lipophilicity

Log $P_{o/w}$ (iLOGP) [?]

iLOGP: in-house
physics-based method
implemented from
Daina A et al. 2014 J.
Chem. Inf. Model.

2.20

Log $P_{o/w}$ (XLOGP3) [?] -0.43

XLOGP3: Atomistic
and knowledge-based

Log S (ESOL) [?]

ESOL: Topological
method implemented
from
Delaney JS. 2004 J.
Chem. Inf. Model.

Water Solubility

-0.56

Solubility
Class [?]

5.58e+01 mg/ml ; 2.76e-01 mol/l

**Solubility class: Log S
scale**
Insoluble < -10 < Poorly
< -6 < Moderately < -4
< Soluble < -2 Very < 0
< Highly

Very soluble

Log S (Ali) [?]

Ali: Topological method
implemented from
Ali J. et al. 2012 J.
Chem. Inf. Model.

-0.09

Solubility
Class [?]

1.64e+02 mg/ml ; 8.11e-01 mol/l

**Solubility class: Log S
scale**
Insoluble < -10 < Poorly
< -6 < Moderately < -4
< Soluble < -2 Very < 0
< Highly

Very soluble

Log S (SILICOS-IT) [?]

SILICOS-IT:
Fragmental method
calculated by
FILTER-IT program,
version 1.0.2, courtesy
of SILICOS-IT,
[http://www.silicos-
it.com](http://www.silicos-it.com)

-0.45

Solubility

7.18e+01 mg/ml ; 3.55e-01 mol/l

[method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.](#)

Log $P_{o/w}$ (WLOGP) [?]

WLOGP: Atomistic method implemented from

[Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.](#)

-1.40

Log $P_{o/w}$ (MLOGP) [?]

MLOGP: Topological method implemented from

[Moriguchi I. et al. 1992 Chem. Pharm. Bull.](#)

[Moriguchi I. et al. 1994 Chem. Pharm. Bull.](#)

[Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.](#)

-0.21

Log $P_{o/w}$ (SILICOS-IT) [?]

SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>

-0.11

Consensus Log $P_{o/w}$ [?]

Consensus Log $P_{o/w}$: Average of all five predictions

0.01

Class [?]

Solubility class: Log S scale

[Insoluble < -10 < Poorly Soluble < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly](#)

Pharmacokinetics

GI absorption [?]

Gastrointestinal absorption: according to the white of the BOILED-Egg Low

BBB permeant [?]

BBB permeation: according to the yolk of the BOILED-Egg No

P-gp substrate [?]

P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). No
10-fold CV: ACC=0.72 / AUC=0.77
External: ACC=0.88 / AUC=0.94

CYP1A2 inhibitor [?]


Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). No
10-fold CV: ACC=0.83 / AUC=0.90
External: ACC=0.84 / AUC=0.91

CYP2C19 inhibitor [?]

Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set). No
10-fold CV: ACC=0.80 / AUC=0.86
External: ACC=0.80 / AUC=0.87

CYP2C9 inhibitor [?]

Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set). No
10-fold CV: ACC=0.78 / AUC=0.85
External: ACC=0.71 / AUC=0.81

CYP2D6 inhibitor **Cytochrome P450 2D6****inhibitor:** [SVM model](#)[built on 3664 molecules](#)[\(training set\)](#)


and tested on 1068 No

[molecules \(test set\)](#)

10-fold CV: ACC=0.79 /

[AUC=0.85](#)

External: ACC=0.81 /

[AUC=0.87](#)CYP3A4 inhibitor **Cytochrome P450 3A4****inhibitor:** [SVM model](#)[built on 7518 molecules](#)[\(training set\)](#)


and tested on 2579 No

[molecules \(test set\)](#)

10-fold CV: ACC=0.77 /

[AUC=0.85](#)


External: ACC=0.78 /

[AUC=0.86](#)Log K_p (skin
permeation) **Skin permeation:**[QSPR model](#)

-7.84 cm/s

[implemented from](#)[Potts RO and Guy RH.](#)[1992 Pharm. Res.](#)

Druglikeness

Lipinski **Lipinski (Pfizer) filter:**[implemented from](#)[Lipinski CA. et al. 2001](#)[Adv. Drug Deliv. Rev.](#)

Yes; 0 violation

[MW < 500](#)[MLOGP < 4.15](#)[N or O < 10](#)[NH or OH < 5](#)Ghose **Ghose filter:**[implemented from](#)[Ghose AK. et al. 1999 J.](#)[Comb. Chem.](#)

No; 1 violation: WLOGP<-0.4


[160 < MW < 480](#)[-0.4 < WLOGP < 5.6](#)[40 < MR < 130](#)[20 < atoms < 70](#)Veber **Veber (GSK) filter:**[implemented from](#)[Veber DF. et al. 2002 J.](#)[Med. Chem.](#)

Yes


[Rotatable bonds < 10](#)[TPSA < 140](#)Egan **Egan (Pharmacia)****filter:** [implemented](#)[from](#)[Egan WJ. et al. 2000 J.](#)[Med. Chem.](#)

Yes

[WLOGP < 5.88](#)[TPSA < 131.6](#)

Muegge **Muegge (Bayer) filter:**

implemented from
[Muegge I. et al. 2001 J. Med. Chem.](#)
 $200 < MW < 600$
 $-2 < XLOGP < 5$
 $TPSA < 150$ Yes
 $Num. rings < 7$
 $Num. carbon > 4$
 $Num. heteroatoms > 1$
 $Num. rotatable bonds < 15$
 $H-bond acc. < 10$
 $H-bond don. < 5$

Bioavailability Score **Abbott Bioavailability**

Score: Probability of F
 $> 10\%$ in rat 0.55
 implemented from
[Martin YC. 2005 J. Med. Chem.](#)

Medicinal Chemistry

PAINS **Pan Assay Interference**


Structures:
 implemented from 0 alert
[Baell JB. & Holloway GA. 2010 J. Med. Chem.](#)

Brenk **Structural Alert:**

implemented from 0 alert
[Brenk R. et al. 2008 ChemMedChem](#)


Leadlikeness **Leadlikeness:**

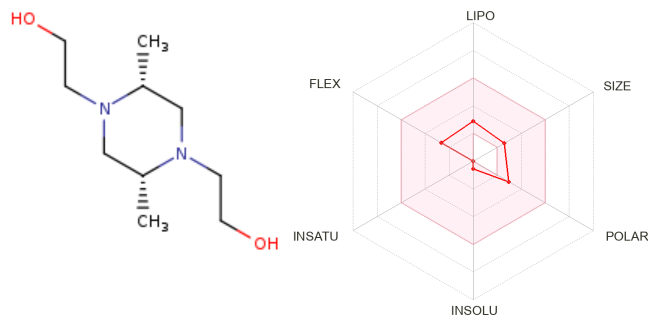
implemented from
[Teague SJ. 1999 Angew. Chem. Int. Ed.](#) No; 1 violation: MW<250
 $250 < MW < 350$
 $XLOGP < 3.5$
 $Num. rotatable bonds < 7$

Synthetic accessibility **Synthetic accessibility**

score: from 1 (very easy) to 10 (very difficult)
 based on 1024
[fragmental contributions \(FP2\) modulated by size and complexity penalties, trained on 12'782'590 molecules and tested on 40 external molecules](#) 2.51
 $(r^2 = 0.94)$

Molecule 16

Water Solubility 



SMILES
S OCCN1C[C@@H](C)N(C[C@H]1C)CCO

Physicochemical Properties

Formula	C10H22N2O2
Molecular weight	202.29 g/mol
Num. heavy atoms	14
Num. arom. heavy atoms	0
Fraction Csp3	1.00
Num. rotatable bonds	4
Num. H-bond acceptors	4
Num. H-bond donors	2
Molar Refractivity	64.02
TPSA	

Topological Polar Surface Area:
Calculated from
Ertl P. et al. 2000 J. Med. Chem.

46.94 Å²

Lipophilicity

Log $P_{o/w}$ (iLOGP)

iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.

2.15

Log $P_{o/w}$ (XLOGP3)

XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry

-0.43

Log $P_{o/w}$ (WLOGP)

WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.

-1.40

Log $P_{o/w}$ (MLOGP)

MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull.

-0.21

Log S (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.

-0.56

Solubility Class

5.58e+01 mg/ml ; 2.76e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Very soluble

Log S (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.

-0.09

Solubility Class

1.64e+02 mg/ml ; 8.11e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Very soluble

Log S (SILICOS-IT)

SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>

-0.45

Solubility Class

7.18e+01 mg/ml ; 3.55e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Soluble

Pharmacokinetics

GI absorption

Gastrointestinal absorption: according to the white of the BOILED-Egg

Low

BBB permeant

BBB permeation: according to the yolk of the BOILED-Egg

No

P-gp substrate

P-glycoprotein substrate: SVM model built on 1033 molecules

No

[Lipinski PA. et al. 2001
Adv. Drug. Deliv. Rev.](#)

Log $P_{o/w}$ (SILICOS-IT)

SILICOS-IT: Hybrid
fragmental/topological
method calculated by
FILTER-IT program, -0.11
version 1.0.2, courtesy
of SILICOS-IT,
[http://www.silicos-
it.com](http://www.silicos-
it.com)

Consensus Log $P_{o/w}$

Consensus Log $P_{o/w}$: 0.00
[Average of all five
predictions](#)

(training set)
and tested on 415
molecules (test set)
10-fold CV: ACC=0.72 /
AUC=0.77
External: ACC=0.88 /
AUC=0.94

CYP1A2 inhibitor

**Cytochrome P450 1A2
inhibitor:** SVM model
built on 9145 molecules
(training set)
and tested on 3000 No
molecules (test set)
10-fold CV: ACC=0.83 /
AUC=0.90
External: ACC=0.84 /
AUC=0.91

CYP2C19 inhibitor

**Cytochrome P450
2C19 inhibitor:** SVM
model built on 9272
molecules (training set). No
and tested on 3000
molecules (test set).
10-fold CV: ACC=0.80 /
AUC=0.86
External: ACC=0.80 /
AUC=0.87

CYP2C9 inhibitor

**Cytochrome P450 2C9
inhibitor:** SVM model
built on 5940 molecules
(training set). No
and tested on 2075
molecules (test set).
10-fold CV: ACC=0.78 /
AUC=0.85
External: ACC=0.71 /
AUC=0.81

CYP2D6 inhibitor

**Cytochrome P450 2D6
inhibitor:** SVM model
built on 3664 molecules
(training set). No
and tested on 1068
molecules (test set).
10-fold CV: ACC=0.79 /
AUC=0.85
External: ACC=0.81 /
AUC=0.87

CYP3A4 inhibitor

**Cytochrome P450 3A4
inhibitor:** SVM model
built on 7518 molecules
(training set). No
and tested on 2579
molecules (test set).
10-fold CV: ACC=0.77 /
AUC=0.85
External: ACC=0.78 /
AUC=0.86

Log K_p (skin
permeation) -7.84 cm/s

Skin permeation:
QSPR model

[implemented from Potts RO and Guy RH. 1992 Pharm. Res.](#)

Druglikeness

Lipinski [?]

Lipinski (Pfizer) filter:

[implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev.](#)
[MW < 500](#)
[MLOGP < 4.15](#)
[N or O < 10](#)
[NH or OH < 5](#)

Yes; 0 violation

Ghose [?]

Ghose filter:

[implemented from Ghose AK. et al. 1999 J. Comb. Chem.](#)
[160 < MW < 480](#)
[-0.4 < WLOGP < 5.6](#)
[40 < MR < 130](#)
[20 < atoms < 70](#)

No; 1 violation: WLOGP < -0.4

Veber [?]

Veber (GSK) filter:

[implemented from Veber DF. et al. 2002 J. Med. Chem.](#)
[Rotatable bonds < 10](#)
[TPSA < 140](#)

Yes

Egan [?]

Egan (Pharmacia) filter: [implemented from](#)

[Egan WJ. et al. 2000 J. Med. Chem.](#)
[WLOGP < 5.88](#)
[TPSA < 131.6](#)

Yes

Muegge [?]

Muegge (Bayer) filter: [implemented from](#)

[Muegge I. et al. 2001 J. Med. Chem.](#)
[200 < MW < 600](#)
[-2 < XLOGP < 5](#)
[TPSA < 150](#)
[Num. rings < 7](#)
[Num. carbon > 4](#)
[Num. heteroatoms > 1](#)
[Num. rotatable bonds < 15](#)
[H-bond acc. < 10](#)
[H-bond don. < 5](#)

Yes

Bioavailability Score [?]

Abbott Bioavailability Score: [Probability of F](#)

[> 10% in rat](#)
[implemented from Martin YC. 2005 J. Med. Chem.](#)

0.55

Medicinal Chemistry

PAINS [?]

0 alert

Pan Assay Interference Structures:

[implemented from Baell JB. & Holloway GA. 2010 J. Med. Chem.](#)

Brenk

Structural Alert:

[implemented from Brenk R. et al. 2008 ChemMedChem](#) 0 alert

Leadlikeness

Leadlikeness:

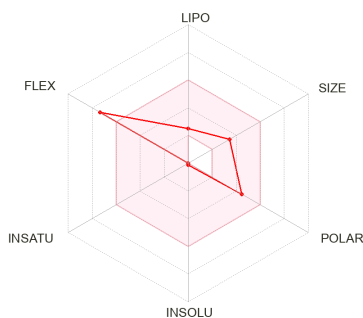
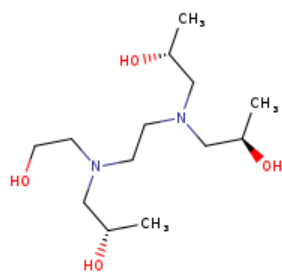
[implemented from Teague SJ. 1999 Angew. Chem. Int. Ed.](#) No; 1 violation: MW<250
[250 < MW < 350](#)
[XLOGP < 3.5](#)
[Num. rotatable bonds < 7](#)

Synthetic accessibility

Synthetic accessibility

score: from 1 (very easy) to 10 (very difficult) based on 1024 fragmental contributions (FP2) modulated by size and complexity penalties, trained on 12'782'590 molecules and tested on 40 external molecules ($r^2 = 0.94$) 2.51

Molecule 17



SMILES OCCN(C[C@@H](O)C)CCN(C[C@H](O)C)C[C@H](O)C

Physicochemical Properties

Formula C13H30N2O4
 Molecular weight 278.39 g/mol
 Num. heavy atoms 19
 Num. arom. heavy atoms 0
 Fraction Csp3 1.00
 Num. rotatable bonds 11
 Num. H-bond acceptors 6
 Num. H-bond donors 4
 Molar Refractivity 75.04
 TPSA 87.40 Å²

Topological Polar

Surface Area:
[Calculated from](#)

Log *S* (ESOL)

ESOL: [Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.](#)

Water Solubility

-0.12

Solubility Class

2.10e+02 mg/ml ; 7.55e-01 mol/l

Solubility class: Log *S* scale
 Insoluble < -10 < Poorly
 < -6 < Moderately < -4
 < Soluble < -2 Very < 0
 < Highly

Log *S* (Ali)

Ali: [Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.](#)

-0.20

Solubility Class

1.74e+02 mg/ml ; 6.26e-01 mol/l
 Very soluble

Solubility class: Log *S* scale
 Insoluble < -10 < Poorly
 < -6 < Moderately < -4

Ertl P. et al. 2000 J. Med. Chem.		< Soluble < -2 Very < 0 < Highly	
Log $P_{o/w}$ (iLOGP)	Lipophilicity	Log S (SILICOS-IT)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	2.47	SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-0.39
Log $P_{o/w}$ (XLOGP3)		Solubility Class	1.13e+02 mg/ml ; 4.06e-01 mol/l
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.	-1.14	Solubility class: Log S scale Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Soluble
Log $P_{o/w}$ (WLOGP)			Pharmacokinetics
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	-1.27	GI absorption	
Log $P_{o/w}$ (MLOGP)		Gastrointestinal absorption: according to the white of the BOILED-Egg	High
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	-0.62	BBB permeant	
Log $P_{o/w}$ (SILICOS-IT)		BBB permeation: according to the yolk of the BOILED-Egg	No
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-0.16	P-gp substrate	
Consensus Log $P_{o/w}$		P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
Consensus Log $P_{o/w}$: Average of all five predictions	-0.14	CYP1A2 inhibitor	
		Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.83 / AUC=0.90 External: ACC=0.84 / AUC=0.91	No
		CYP2C19 inhibitor	
		Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.80 / AUC=0.86 External: ACC=0.80 / AUC=0.87	No

CYP2C9 inhibitor ⓘ

Cytochrome P450 2C9**inhibitor:** SVM model

built on 5940 molecules

(training set)

and tested on 2075 No

molecules (test set)

10-fold CV: ACC=0.78 /

AUC=0.85

External: ACC=0.71 /

AUC=0.81

CYP2D6 inhibitor ⓘ

Cytochrome P450 2D6**inhibitor:** SVM model

built on 3664 molecules

(training set)

and tested on 1068 No

molecules (test set)

10-fold CV: ACC=0.79 /

AUC=0.85

External: ACC=0.81 /

AUC=0.87

CYP3A4 inhibitor ⓘ

Cytochrome P450 3A4**inhibitor:** SVM model

built on 7518 molecules

(training set)

and tested on 2579 No

molecules (test set)

10-fold CV: ACC=0.77 /

AUC=0.85

External: ACC=0.78 /

AUC=0.86

Log K_p (skin
permeation) ⓘ**Skin permeation:**

QSPR model

-8.81 cm/s

implemented from

Potts RO and Guy RH.

1992 Pharm. Res.

Druglikeness

Lipinski ⓘ

Lipinski (Pfizer) filter:

implemented from

Lipinski CA. et al. 2001

Adv. Drug Deliv. Rev. Yes; 0 violation

MW < 500

MLOGP < 4.15

N or O < 10

NH or OH < 5

Ghose ⓘ

Ghose filter:

implemented from

Ghose AK. et al. 1999 J.

Comb. Chem.

No; 1 violation: WLOGP<-0.4

160 < MW < 480

-0.4 < WLOGP < 5.6

40 < MR < 130

20 < atoms < 70

Veber ⓘ

No; 1 violation: Rotors>10

Veber (GSK) filter:

implemented from

Veber DE. et al. 2002 J.

Med. Chem.

[Rotatable bonds < 10](#)
[TPSA < 140](#)

Egan

Egan (Pharmacia)

filter: [implemented](#)

[from](#)
[Egan W.J. et al. 2000 J. Med. Chem.](#) Yes
[WLOGP < 5.88](#)
[TPSA < 131.6](#)

Muegge

Muegge (Bayer) filter:

[implemented from](#)

[Muegge I. et al. 2001 J. Med. Chem.](#) Yes
[200 < MW < 600](#)
[-2 < XLOGP < 5](#)
[TPSA < 150](#)
[Num. rings < 7](#)
[Num. carbon > 4](#)
[Num. heteroatoms > 1](#)
[Num. rotatable bonds < 15](#)
[H-bond acc. < 10](#)
[H-bond don. < 5](#)

Bioavailability Score

Abbott Bioavailability

Score: [Probability of F > 10% in rat](#) 0.55
[implemented from](#)
[Martin Y.C. 2005 J. Med. Chem.](#)

Medicinal Chemistry

PAINS

Pan Assay Interference

Structures:

[implemented from](#) 0 alert
[Baell JB. & Holloway GA. 2010 J. Med. Chem.](#)

Brenk

Structural Alert:

[implemented from](#) 0 alert
[Brenk R. et al. 2008 ChemMedChem](#)

Leadlikeness

Leadlikeness:

[implemented from](#)
[Teague S.J. 1999 Angew. Chem. Int. Ed.](#) No; 1 violation: Rotors>7
[250 < MW < 350](#)
[XLOGP < 3.5](#)
[Num. rotatable bonds < 7](#)

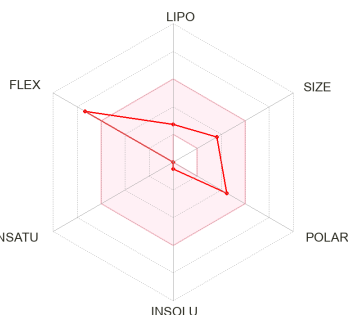
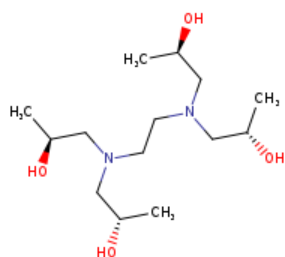
Synthetic accessibility 3.18

Synthetic accessibility

score: [from 1 \(very easy\) to 10 \(very difficult\)](#)
[based on 1024 fragmental contributions \(FP2\) modulated by size and complexity penalties.](#)

trained on 12'782'590
molecules and tested on
40 external molecules
($r^2 = 0.94$)

Molecule 18



SMILES C[C@H](CN(C[C@@H](O)C)CCN(C[C@@H](O)C)[C@@H](O)C

Physicochemical Properties

Formula C14H32N2O4
Molecular weight 292.41 g/mol
Num. heavy atoms 20
Num. arom. heavy atoms 0
Fraction Csp3 1.00
Num. rotatable bonds 11
Num. H-bond acceptors 6
Num. H-bond donors 4
Molar Refractivity 79.85
TPSA Å^2

Topological Polar Surface Area:
Calculated from
Ertl P. et al. 2000 J. Med. Chem.

87.40 Å^2

Lipophilicity

Log $P_{o/w}$ (iLOGP) Å^2

iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.

3.04

Log $P_{o/w}$ (XLOGP3)

XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.

-0.70

Log $P_{o/w}$ (WLOGP)

WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.

-0.89

Log S (ESOL)

ESOL: Topological method implemented from Delaney JS. 2004 J. Chem. Inf. Model.

Water Solubility

-0.49

Solubility Class

9.55e+01 mg/ml ; 3.27e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Very soluble

Log S (Ali)

Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.

-0.66

Solubility Class

6.39e+01 mg/ml ; 2.19e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Very soluble

Log S (SILICOS-IT)

SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>

-0.42

Solubility Class

1.12e+02 mg/ml ; 3.82e-01 mol/l

Solubility class: Log S scale
Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly


Soluble

Pharmacokinetics


GI absorption

Gastrointestinal absorption: according to the white of the BOILED-Egg


High

Log $P_{o/w}$ (MLOGP) **MLOGP: Topological method implemented from**


[Moriguchi I. et al. 1992 Chem. Pharm. Bull.](#) -0.35
[Moriguchi I. et al. 1994 Chem. Pharm. Bull.](#)
[Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.](#)

Log $P_{o/w}$ (SILICOS-IT) 


SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com> 0.09

Consensus Log $P_{o/w}$ 


Consensus Log $P_{o/w}$: Average of all five predictions 0.24

BBB permeant 


BBB permeation: according to the yolk of the BOILED-Egg No

P-gp substrate 


P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set) No
 10-fold CV: ACC=0.72 / AUC=0.77
 External: ACC=0.88 / AUC=0.94

CYP1A2 inhibitor 


Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set) No
 10-fold CV: ACC=0.83 / AUC=0.90
 External: ACC=0.84 / AUC=0.91

CYP2C19 inhibitor 


Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) No
 10-fold CV: ACC=0.80 / AUC=0.86
 External: ACC=0.80 / AUC=0.87

CYP2C9 inhibitor 

Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) No
 10-fold CV: ACC=0.78 / AUC=0.85
 External: ACC=0.71 / AUC=0.81


CYP2D6 inhibitor 

Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) No
 10-fold CV: ACC=0.79 / AUC=0.85
 External: ACC=0.81 / AUC=0.87

CYP3A4 inhibitor  No

Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set)

and tested on 2579
 molecules (test set)
 10-fold CV: ACC=0.77 /
 AUC=0.85
 External: ACC=0.78 /
 AUC=0.86

Log K_p (skin
 permeation) 

Skin permeation:

[QSPR model](#) -8.58 cm/s
 implemented from
[Potts RO and Guy RH.](#)
[1992 Pharm. Res.](#)

Druglikeness

Lipinski 

Lipinski (Pfizer) filter:

implemented from
[Lipinski CA. et al. 2001](#)
[Adv. Drug Deliv. Rev.](#) Yes; 0 violation
 MW < 500
 MLOGP < 4.15
 N or O < 10
 NH or OH < 5

Ghose 

Ghose filter:

implemented from
[Ghose AK. et al. 1999 J.](#)
[Comb. Chem.](#) No; 1 violation: WLOGP<-0.4
 160 < MW < 480
 -0.4 < WLOGP < 5.6
 40 < MR < 130
 20 < atoms < 70

Veber 


Veber (GSK) filter:

implemented from
[Veber DF. et al. 2002 J.](#) No; 1 violation: Rotors>10
[Med. Chem.](#)
 Rotatable bonds < 10
 TPSA < 140

Egan 

**Egan (Pharmacia)
 filter:** implemented

from
[Egan WJ. et al. 2000 J.](#) Yes
[Med. Chem.](#)
 WLOGP < 5.88
 TPSA < 131.6

Muegge 

Muegge (Bayer) filter:

implemented from
[Muegge I. et al. 2001 J.](#)
[Med. Chem.](#)
 200 < MW < 600
 -2 < XLOGP < 5
 TPSA < 150 Yes
 Num. rings < 7
 Num. carbon > 4
 Num. heteroatoms > 1
 Num. rotatable bonds <
 15
 H-bond acc. < 10
 H-bond don. < 5

Bioavailability Score

Abbott Bioavailability:**Score:** Probability of F

> 10% in rat 0.55

implemented from

[Martin YC. 2005 J.](#)[Med. Chem.](#)

Medicinal Chemistry

PAINS

Pan Assay Interference**Structures:**

implemented from

0 alert

[Baell JB. & Holloway](#)[GA. 2010 J. Med.](#)[Chem.](#)

Brenk

Structural Alert:

implemented from

0 alert

[Brenk R. et al. 2008](#)[ChemMedChem](#)

Leadlikeness

Leadlikeness:

implemented from

[Teague SJ. 1999 Angew.](#)[Chem. Int. Ed.](#)

No; 1 violation: Rotors>7

[250 < MW < 350](#)[XLOGP < 3.5](#)[Num. rotatable bonds <](#)[7](#)

Synthetic accessibility

Synthetic accessibility**score:** from 1 (very

easy) to 10 (very

difficult)

based on 1024

fragmental contributions 3.44

(FP2) modulated by size

and complexity penalties.

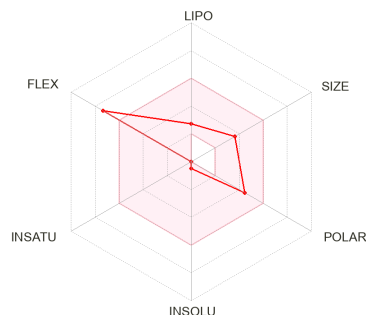
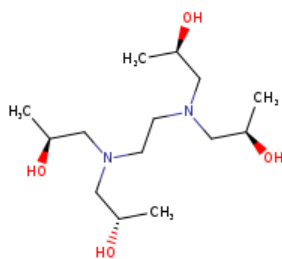
trained on 12'782'590

molecules and tested on

40 external molecules

(r² = 0.94)

Molecule 19



Log S (ESOL)

ESOL: Topological**method implemented****from**[Delaney JS. 2004 J.](#)[Chem. Inf. Model.](#)

Water Solubility

-0.49

Solubility

9.55e+01 mg/ml ; 3.27e-01 mol/l

Class

Solubility class: Log S**scale**[Insoluble < -10 < Poorly](#) Very soluble[< -6 < Moderately < -4](#)[< Soluble < -2 Very < 0](#)[< Highly](#)SMILE C[C@H](CN(C[C@H](O)C)CCN(C[C@@H](O)C)[C@H](O)C)

Physicochemical Properties


Formula C₁₄H₃₂N₂O₄

Molecular weight 292.41 g/mol


Num. heavy atoms 20

Num. arom. heavy atoms	0	Log <i>S</i> (Ali)	
Fraction Csp3	1.00	Ali: Topological method implemented from Ali J. et al. 2012 J. Chem. Inf. Model.	-0.66
Num. rotatable bonds	11		
Num. H-bond acceptors	6		
Num. H-bond donors	4		
Molar Refractivity	79.85	Solubility Class	6.39e+01 mg/ml ; 2.19e-01 mol/l
TPSA		Solubility class: Log <i>S</i> scale	
Topological Polar Surface Area: Calculated from Ertl P. et al. 2000 J. Med. Chem.	87.40 Å ²	Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	Very soluble
	Lipophilicity		
Log <i>P</i> _{o/w} (iLOGP)		Log <i>S</i> (SILICOS-IT)	
iLOGP: in-house physics-based method implemented from Daina A et al. 2014 J. Chem. Inf. Model.	3.03	SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	-0.42
Log <i>P</i> _{o/w} (XLOGP3)		Solubility Class	1.12e+02 mg/ml ; 3.82e-01 mol/l
XLOGP3: Atomistic and knowledge-based method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.	-0.70	Solubility class: Log <i>S</i> scale	Soluble
Log <i>P</i> _{o/w} (WLOGP)		Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly	
WLOGP: Atomistic method implemented from Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.	-0.89		Pharmacokinetics
Log <i>P</i> _{o/w} (MLOGP)		GI absorption	
MLOGP: Topological method implemented from Moriguchi I. et al. 1992 Chem. Pharm. Bull. Moriguchi I. et al. 1994 Chem. Pharm. Bull. Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.	-0.35	Gastrointestinal absorption: according to the white of the BOILED-Egg	High
Log <i>P</i> _{o/w} (SILICOS-IT)		BBB permeant	
SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, http://www.silicos-it.com	0.09	BBB permeation: according to the yolk of the BOILED-Egg	No
Consensus Log <i>P</i> _{o/w}		P-gp substrate	
Consensus Log <i>P</i>_{o/w}: Average of all five predictions	0.24	P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). 10-fold CV: ACC=0.72 / AUC=0.77 External: ACC=0.88 / AUC=0.94	No
		CYP1A2 inhibitor	No
		Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). 10-fold CV: ACC=0.83 / AUC=0.90	


[External: ACC=0.84 / AUC=0.91](#)

CYP2C19 inhibitor 


Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set) No
 10-fold CV: ACC=0.80 / AUC=0.86
 External: ACC=0.80 / AUC=0.87

CYP2C9 inhibitor 


Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set) No
 10-fold CV: ACC=0.78 / AUC=0.85
 External: ACC=0.71 / AUC=0.81

CYP2D6 inhibitor 

Cytochrome P450 2D6 inhibitor: SVM model built on 3664 molecules (training set) and tested on 1068 molecules (test set) No
 10-fold CV: ACC=0.79 / AUC=0.85
 External: ACC=0.81 / AUC=0.87

CYP3A4 inhibitor 

Cytochrome P450 3A4 inhibitor: SVM model built on 7518 molecules (training set) and tested on 2579 molecules (test set) No
 10-fold CV: ACC=0.77 / AUC=0.85
 External: ACC=0.78 / AUC=0.86

Log K_p (skin permeation) 

Skin permeation: QSPR model implemented from Potts RO and Guy RH. 1992 Pharm. Res. -8.58 cm/s

Druglikeness

Lipinski 

Lipinski (Pfizer) filter: implemented from Lipinski CA. et al. 2001 Adv. Drug Deliv. Rev. Yes; 0 violation
 MW < 500
 MLOGP < 4.15
 N or O < 10
 NH or OH < 5

Ghose ?

Ghose filter:

implemented from

[Ghose AK. et al. 1999 J.](#)[Comb. Chem.](#)[160 < MW < 480](#)[-0.4 < WLOGP < 5.6](#)[40 < MR < 130](#)[20 < atoms < 70](#)

No; 1 violation: WLOGP<-0.4

Veber ?

Veber (GSK) filter:

implemented from

[Veber DF. et al. 2002 J.](#)[Med. Chem.](#)[Rotatable bonds < 10](#)[TPSA < 140](#)

No; 1 violation: Rotors>10

Egan ?

Egan (Pharmacia)**filter:** implemented

from

[Egan WJ. et al. 2000 J.](#)[Med. Chem.](#)[WLOGP < 5.88](#)[TPSA < 131.6](#)

Yes

Muegge ?

Muegge (Bayer) filter:

implemented from

[Muegge I. et al. 2001 J.](#)[Med. Chem.](#)[200 < MW < 600](#)[-2 < XLOGP < 5](#)[TPSA < 150](#)[Num. rings < 7](#)[Num. carbon > 4](#)[Num. heteroatoms > 1](#)[Num. rotatable bonds <](#)[15](#)[H-bond acc. < 10](#)[H-bond don. < 5](#)

Yes

Bioavailability Score ?

Abbott Bioavailability**Score:** Probability of F[> 10% in rat](#)

implemented from

[Martin YC. 2005 J.](#)[Med. Chem.](#)

0.55

Medicinal Chemistry

PAINS ?

Pan Assay Interference**Structures:**

implemented from

[Baell JB. & Holloway.](#)[GA. 2010 J. Med.](#)[Chem.](#)

0 alert

Brenk ?

Structural Alert:

implemented from

[Brenk R. et al. 2008](#)[ChemMedChem](#)

0 alert

Leadlikeness ?

No; 1 violation: Rotors>7

Leadlikeness:

implemented from

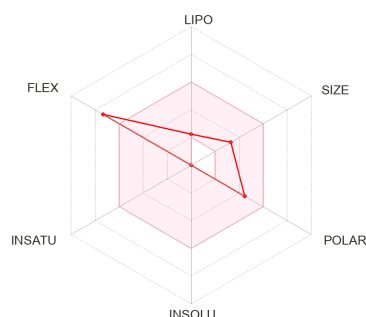
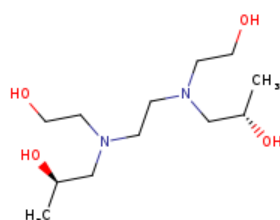
[Teague SJ. 1999 Angew. Chem. Int. Ed.](#)
[250 < MW < 350](#)
[XLOGP < 3.5](#)
[Num. rotatable bonds < 7](#)

Synthetic accessibility

Synthetic accessibility

score: from 1 (very easy) to 10 (very difficult)
 based on 1024 fragmental contributions 3.44
 (FP2) modulated by size and complexity penalties, trained on 12'782'590 molecules and tested on 40 external molecules
 ($r^2 = 0.94$)

Molecule 20



SMILES OCCN(C[C@H](O)C)CCN(C[C@@H](O)C)CCO

Physicochemical Properties

Formula C12H28N2O4
 Molecular weight 264.36 g/mol
 Num. heavy atoms 18
 Num. arom. heavy atoms 0
 Fraction Csp3 1.00
 Num. rotatable bonds 11
 Num. H-bond acceptors 6
 Num. H-bond donors 4
 Molar Refractivity 70.24
 TPSA

Topological Polar Surface Area:
 Calculated from [Ertl P. et al. 2000 J. Med. Chem.](#)

87.40 Å²

Lipophilicity

Log $P_{o/w}$ (iLOGP)

iLOGP: in-house physics-based method implemented from [Daina A et al. 2014 J. Chem. Inf. Model.](#)

2.32

Log $P_{o/w}$ (XLOGP3)

XLOGP3: Atomistic and knowledge-based

-1.57

Log S (ESOL)

ESOL: Topological method implemented from [Delaney JS. 2004 J. Chem. Inf. Model.](#)

Water Solubility

0.24

Solubility Class

4.55e+02 mg/ml ; 1.72e+00 mol/l

Solubility class: Log S scale

Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Highly soluble

Log S (Ali)

Ali: Topological method implemented from [Ali J. et al. 2012 J. Chem. Inf. Model.](#)

0.24

Solubility Class

4.62e+02 mg/ml ; 1.75e+00 mol/l

Solubility class: Log S scale

Insoluble < -10 < Poorly < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly

Highly soluble

Log S (SILICOS-IT)

SILICOS-IT: Fragmental method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>

-0.37

Solubility

1.14e+02 mg/ml ; 4.31e-01 mol/l

[method calculated by XLOGP program, version 3.2.2, courtesy of CCBG, Shanghai Institute of Organic Chemistry.](#)

Log $P_{o/w}$ (WLOGP) [?]

WLOGP: Atomistic method implemented from

-1.66

[Wildman SA and Crippen GM. 1999 J. Chem. Inf. Model.](#)

Log $P_{o/w}$ (MLOGP) [?]

MLOGP: Topological method implemented from

-0.89

[Moriguchi I. et al. 1992 Chem. Pharm. Bull.](#)
[Moriguchi I. et al. 1994 Chem. Pharm. Bull.](#)
[Lipinski PA. et al. 2001 Adv. Drug. Deliv. Rev.](#)

Log $P_{o/w}$ (SILICOS-IT) [?]

SILICOS-IT: Hybrid fragmental/topological method calculated by FILTER-IT program, version 1.0.2, courtesy of SILICOS-IT, <http://www.silicos-it.com>

-0.41

Consensus Log $P_{o/w}$ [?]

Consensus Log $P_{o/w}$: Average of all five predictions

-0.44

Class [?]

Solubility class: Log S scale

[Insoluble < -10 < Poorly Soluble < -6 < Moderately < -4 < Soluble < -2 Very < 0 < Highly](#)

Pharmacokinetics

GI absorption [?]

Gastrointestinal absorption: according to the white of the BOILED-Egg High

BBB permeant [?]

BBB permeation: according to the yolk of the BOILED-Egg No

P-gp substrate [?]

P-glycoprotein substrate: SVM model built on 1033 molecules (training set) and tested on 415 molecules (test set). No
10-fold CV: ACC=0.72 / AUC=0.77
External: ACC=0.88 / AUC=0.94

CYP1A2 inhibitor [?]


Cytochrome P450 1A2 inhibitor: SVM model built on 9145 molecules (training set) and tested on 3000 molecules (test set). No
10-fold CV: ACC=0.83 / AUC=0.90
External: ACC=0.84 / AUC=0.91

CYP2C19 inhibitor [?]

Cytochrome P450 2C19 inhibitor: SVM model built on 9272 molecules (training set) and tested on 3000 molecules (test set). No
10-fold CV: ACC=0.80 / AUC=0.86
External: ACC=0.80 / AUC=0.87

CYP2C9 inhibitor [?]

Cytochrome P450 2C9 inhibitor: SVM model built on 5940 molecules (training set) and tested on 2075 molecules (test set). No
10-fold CV: ACC=0.78 / AUC=0.85
External: ACC=0.71 / AUC=0.81

CYP2D6 inhibitor **Cytochrome P450 2D6****inhibitor:** [SVM model](#)[built on 3664 molecules](#)[\(training set\)](#)


and tested on 1068 No

[molecules \(test set\)](#)

10-fold CV: ACC=0.79 /

[AUC=0.85](#)

External: ACC=0.81 /

[AUC=0.87](#)CYP3A4 inhibitor **Cytochrome P450 3A4****inhibitor:** [SVM model](#)[built on 7518 molecules](#)[\(training set\)](#)


and tested on 2579 No

[molecules \(test set\)](#)

10-fold CV: ACC=0.77 /

[AUC=0.85](#)

External: ACC=0.78 /


[AUC=0.86](#)Log K_p (skin
permeation) **Skin permeation:**[QSPR model](#)

-9.03 cm/s

implemented from

[Potts RO and Guy RH.](#)[1992 Pharm. Res.](#)

Druglikeness

Lipinski **Lipinski (Pfizer) filter:**

implemented from

[Lipinski CA. et al. 2001](#)[Adv. Drug Deliv. Rev.](#)

Yes; 0 violation

[MW < 500](#)[MLOGP < 4.15](#)[N or O < 10](#)[NH or OH < 5](#)Ghose **Ghose filter:**

implemented from

[Ghose AK. et al. 1999 J.](#)[Comb. Chem.](#)

No; 1 violation: WLOGP<-0.4

[160 < MW < 480](#)[-0.4 < WLOGP < 5.6](#)[40 < MR < 130](#)[20 < atoms < 70](#)Veber **Veber (GSK) filter:**

implemented from

[Veber DF. et al. 2002 J.](#)[Med. Chem.](#)

No; 1 violation: Rotors>10


[Rotatable bonds < 10](#)[TPSA < 140](#)Egan **Egan (Pharmacia)****filter:** implemented

from


[Egan WJ. et al. 2000 J.](#)[Med. Chem.](#)

Yes

[WLOGP < 5.88](#)[TPSA < 131.6](#)

Muegge **Muegge (Bayer) filter:**

implemented from
[Muegge I. et al. 2001 J. Med. Chem.](#)
[200 < MW < 600](#)
[-2 < XLOGP < 5](#)
[TPSA < 150](#) Yes
[Num. rings < 7](#)
[Num. carbon > 4](#)
[Num. heteroatoms > 1](#)
[Num. rotatable bonds < 15](#)
[H-bond acc. < 10](#)
[H-bond don. < 5](#)

Bioavailability Score **Abbott Bioavailability**

Score: Probability of F
[> 10% in rat](#) 0.55
 implemented from
[Martin YC. 2005 J. Med. Chem.](#)

Medicinal Chemistry

PAINS **Pan Assay Interference****Structures:**


implemented from 0 alert
[Baell JB. & Holloway GA. 2010 J. Med. Chem.](#)

Brenk **Structural Alert:**

implemented from 0 alert
[Brenk R. et al. 2008 ChemMedChem](#)

Leadlikeness **Leadlikeness:**

implemented from
[Teague SJ. 1999 Angew. Chem. Int. Ed.](#) No; 1 violation: Rotors>7
[250 < MW < 350](#)
[XLOGP < 3.5](#)
[Num. rotatable bonds < 7](#)

Synthetic accessibility **Synthetic accessibility**

score: from 1 (very easy) to 10 (very difficult)
 based on 1024
[fragmental contributions](#) 2.84
[\(FP2\) modulated by size and complexity penalties,](#)
[trained on 12'782'590 molecules and tested on 40 external molecules](#)
[\(r² = 0.94\)](#)